



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:21 AM UTC

PDB ID : 2ZII / pdb_00002zii
Title : Crystal Structure of Yeast Vps74-N-term Truncation Variant
Authors : Schmitz, K.R.; Li, S.; Setty, T.G.; Ferguson, K.M.
Deposited on : 2008-02-18
Resolution : 3.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

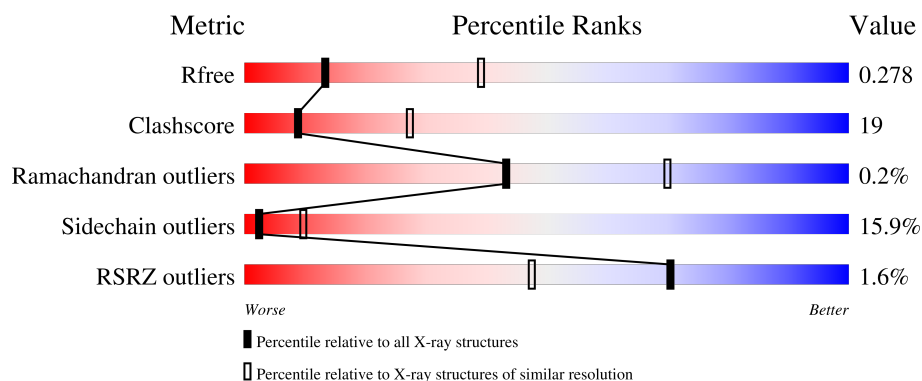
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	288	% 62% 29% 6% .
1	B	288	2% 57% 33% 7% .
1	C	288	2% 58% 31% 7% .
1	D	288	% 64% 27% 6% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8590 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 Vacuolar protein sorting-associated protein 74.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2149	1365	356	416	12			
1	B	281	Total	C	N	O	S	0	0	0
			2126	1348	356	411	11			
1	C	279	Total	C	N	O	S	0	0	0
			2125	1351	355	408	11			
1	D	283	Total	C	N	O	S	0	0	0
			2188	1391	371	414	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLY	-	expression tag	UNP Q06385
A	59	SER	-	expression tag	UNP Q06385
B	58	GLY	-	expression tag	UNP Q06385
B	59	SER	-	expression tag	UNP Q06385
C	58	GLY	-	expression tag	UNP Q06385
C	59	SER	-	expression tag	UNP Q06385
D	58	GLY	-	expression tag	UNP Q06385
D	59	SER	-	expression tag	UNP Q06385

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	D	1	Total	O	0	0
			1	1		

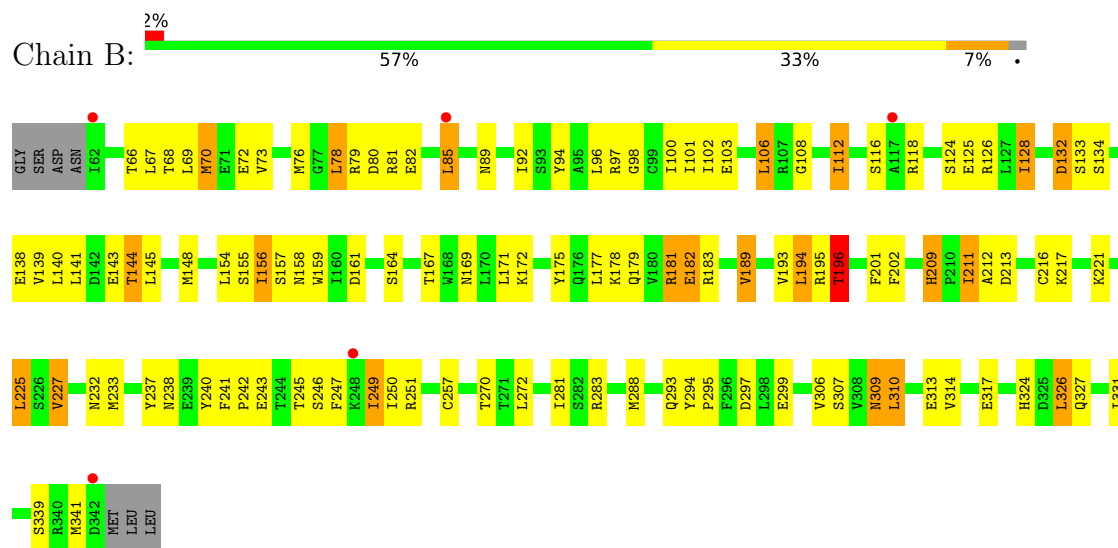
3 Residue-property plots

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.

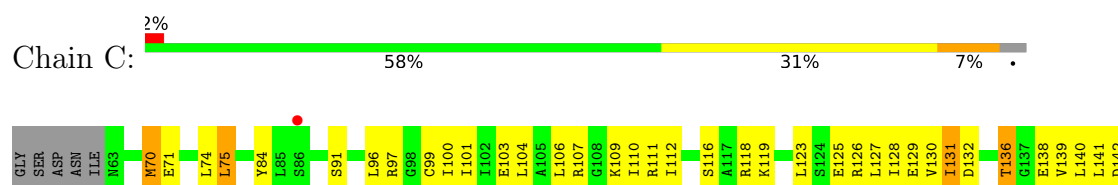
• Molecule 1: Vacuolar protein sorting-associated protein 74

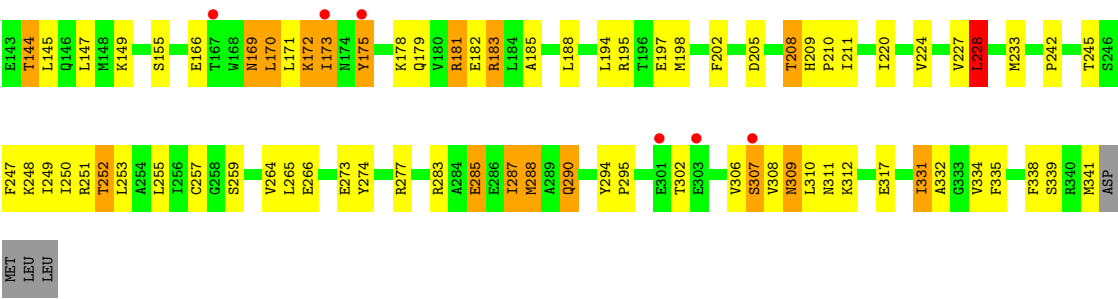


• Molecule 1: Vacuolar protein sorting-associated protein 74

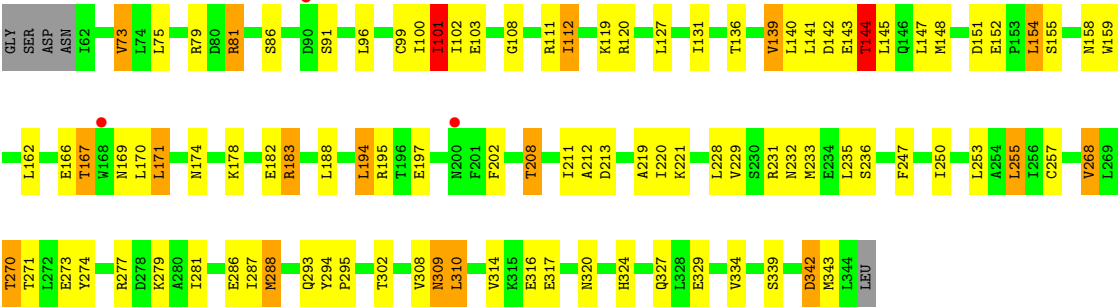


• Molecule 1: Vacuolar protein sorting-associated protein 74





● Molecule 1: Vacuolar protein sorting-associated protein 74



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.08Å 104.08Å 292.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.10 – 3.05 49.10 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.10-3.05) 99.7 (49.10-3.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.220 , 0.281 0.219 , 0.278	Depositor DCC
R_{free} test set	1790 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8590	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 22.79 % 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 5.3113e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	1/2180 (0.0%)	1.13	6/2959 (0.2%)
1	B	0.79	0/2157	1.10	6/2934 (0.2%)
1	C	0.80	0/2156	1.16	15/2929 (0.5%)
1	D	0.87	1/2218 (0.0%)	1.13	5/3005 (0.2%)
All	All	0.83	2/8711 (0.0%)	1.13	32/11827 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	101	ILE	CA-CB	6.53	1.62	1.54
1	A	211	ILE	CA-CB	5.08	1.60	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	175	TYR	N-CA-C	8.52	123.83	112.25
1	A	341	MET	N-CA-C	7.43	121.45	112.38
1	C	172	LYS	N-CA-C	-7.42	96.77	108.63
1	A	170	LEU	N-CA-C	7.04	122.91	111.37
1	A	180	VAL	N-CA-C	6.48	116.64	110.42
1	D	91	SER	N-CA-C	6.18	117.71	110.97
1	C	131	ILE	CB-CA-C	6.16	120.34	111.65
1	C	302	THR	N-CA-C	6.12	119.46	109.24
1	D	101	ILE	CB-CA-C	6.03	119.91	112.02
1	C	274	TYR	N-CA-C	5.97	118.56	111.33
1	A	274	TYR	N-CA-C	5.88	119.56	112.38
1	D	274	TYR	N-CA-C	5.84	117.64	111.28
1	B	195	ARG	CB-CA-C	-5.80	100.42	112.44
1	B	98	GLY	N-CA-C	-5.78	105.80	112.50
1	C	228	LEU	N-CA-C	5.67	121.47	113.02
1	C	170	LEU	N-CA-C	5.59	122.70	110.80
1	D	270	THR	N-CA-C	5.51	118.05	111.71
1	C	170	LEU	CB-CA-C	-5.44	99.59	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	SER	N-CA-C	-5.42	106.67	113.72
1	A	166	GLU	N-CA-C	5.38	119.33	112.87
1	C	228	LEU	CA-CB-CG	5.32	134.93	116.30
1	D	144	THR	N-CA-C	-5.30	105.56	112.23
1	A	169	ASN	N-CA-C	5.20	117.22	108.96
1	B	196	THR	N-CA-C	5.20	116.79	107.80
1	B	89	ASN	N-CA-C	5.18	115.08	108.24
1	C	175	TYR	CA-CB-CG	5.14	123.15	113.90
1	C	290	GLN	N-CA-C	-5.14	105.68	111.28
1	C	334	VAL	N-CA-C	-5.08	105.46	111.00
1	C	228	LEU	CA-C-N	-5.04	117.47	122.77
1	C	228	LEU	C-N-CA	-5.04	117.47	122.77
1	B	209	HIS	CA-C-N	-5.00	115.41	120.31
1	B	209	HIS	C-N-CA	-5.00	115.41	120.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2149	0	2079	81	0
1	B	2126	0	2026	97	0
1	C	2125	0	2049	78	0
1	D	2188	0	2162	68	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
All	All	8590	0	8316	314	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 19.

All (314) 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:B:94:TYR:HD2	1:B:341:MET:HE2	1.10	1.08
1:C:233:MET:HE1	1:C:310:LEU:HD13	1.19	1.08
1:B:106:LEU:HD13	1:B:331:ILE:HD11	1.35	1.05
1:A:242:PRO:HD2	1:A:245:THR:CG2	1.87	1.04
1:C:233:MET:HE1	1:C:310:LEU:CD1	1.90	1.02
1:B:94:TYR:CD2	1:B:341:MET:HE2	2.01	0.95
1:C:100:ILE:HG21	1:C:144:THR:HG21	1.50	0.92
1:D:309:ASN:H	1:D:309:ASN:HD22	1.18	0.91
1:C:233:MET:CE	1:C:310:LEU:HD13	2.07	0.84
1:D:324:HIS:HD2	1:D:327:GLN:OE1	1.62	0.83
1:A:242:PRO:HD2	1:A:245:THR:HG21	1.60	0.82
1:C:70:MET:HE3	1:C:70:MET:H	1.44	0.82
1:B:194:LEU:HD13	1:B:209:HIS:HB3	1.59	0.81
1:A:68:THR:HB	1:A:70:MET:HE3	1.62	0.81
1:C:198:MET:HE1	1:C:205:ASP:HB3	1.61	0.81
1:B:106:LEU:CD1	1:B:331:ILE:HD11	2.12	0.80
1:D:233:MET:H	1:D:309:ASN:HD21	1.28	0.80
1:D:288:MET:HE1	1:D:339:SER:HA	1.65	0.79
1:B:155:SER:OG	1:B:158:ASN:HB2	1.83	0.79
1:D:101:ILE:HD11	1:D:334:VAL:HG22	1.65	0.79
1:B:257:CYS:SG	1:B:288:MET:HE3	2.23	0.78
1:D:101:ILE:HD11	1:D:334:VAL:CG2	2.13	0.78
1:C:309:ASN:HD22	1:C:309:ASN:H	1.33	0.76
1:C:136:THR:HG23	1:C:138:GLU:H	1.51	0.75
1:D:79:ARG:HG3	1:D:86:SER:OG	1.87	0.74
1:A:136:THR:HG21	1:A:141:LEU:HB2	1.70	0.74
1:B:242:PRO:HD2	1:B:245:THR:CG2	2.19	0.73
1:A:79:ARG:HG3	1:A:86:SER:OG	1.89	0.72
1:A:178:LYS:O	1:A:183:ARG:NH1	2.22	0.72
1:C:309:ASN:H	1:C:309:ASN:ND2	1.87	0.72
1:B:189:VAL:HG23	1:B:194:LEU:HD12	1.72	0.72
1:A:242:PRO:HB2	1:A:244:THR:HB	1.72	0.72
1:D:100:ILE:HG21	1:D:144:THR:HG21	1.73	0.71
1:B:81:ARG:NH1	1:D:167:THR:O	2.24	0.71
1:B:309:ASN:H	1:B:309:ASN:HD22	1.36	0.70
1:C:283:ARG:HE	1:C:307:SER:HB2	1.56	0.70
1:B:97:ARG:HG3	1:B:164:SER:HB3	1.74	0.70
1:C:283:ARG:HE	1:C:307:SER:CB	2.06	0.69
1:D:270:THR:HA	1:D:277:ARG:HD3	1.74	0.69
1:C:100:ILE:CG2	1:C:144:THR:HG21	2.20	0.69
1:A:100:ILE:HG21	1:A:144:THR:HG21	1.74	0.69
1:B:118:ARG:HD2	1:B:126:ARG:HD3	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:O	1:B:314:VAL:HG23	1.92	0.69
1:C:208:THR:HG23	1:C:210:PRO:HD3	1.76	0.68
1:B:309:ASN:H	1:B:309:ASN:ND2	1.91	0.68
1:D:257:CYS:SG	1:D:288:MET:HG2	2.34	0.68
1:B:108:GLY:HA2	1:B:327:GLN:HE21	1.60	0.67
1:C:197:GLU:HB3	1:C:208:THR:HG22	1.75	0.67
1:B:242:PRO:HD2	1:B:245:THR:HG21	1.75	0.66
1:B:238:ASN:OD1	1:B:241:PHE:N	2.26	0.66
1:C:198:MET:CE	1:C:205:ASP:HB3	2.24	0.66
1:D:197:GLU:O	1:D:208:THR:HB	1.96	0.65
1:C:169:ASN:C	1:C:169:ASN:HD22	2.04	0.65
1:C:220:ILE:HG23	1:C:255:LEU:HD21	1.79	0.65
1:B:194:LEU:HA	1:B:212:ALA:H	1.62	0.65
1:A:196:THR:HB	1:A:209:HIS:HD2	1.62	0.64
1:B:237:TYR:CD2	1:B:243:GLU:HA	2.32	0.64
1:C:147:LEU:HD22	1:C:175:TYR:CD1	2.32	0.64
1:A:218:GLU:OE2	1:A:218:GLU:HA	1.97	0.64
1:B:69:LEU:O	1:B:73:VAL:HG23	1.98	0.64
1:A:70:MET:CE	1:A:70:MET:H	2.11	0.63
1:A:242:PRO:O	1:A:245:THR:HG23	1.98	0.63
1:A:111:ARG:NH1	1:A:129:GLU:OE1	2.32	0.62
1:D:188:LEU:HB3	1:D:194:LEU:HD22	1.81	0.62
1:B:227:VAL:O	1:B:307:SER:HB2	2.00	0.62
1:C:283:ARG:HH21	1:C:307:SER:HB3	1.65	0.62
1:D:140:LEU:O	1:D:144:THR:HG23	1.99	0.61
1:A:70:MET:H	1:A:70:MET:HE2	1.64	0.61
1:D:247:PHE:HB3	1:D:250:ILE:HB	1.82	0.61
1:B:189:VAL:HG23	1:B:194:LEU:CD1	2.31	0.61
1:C:233:MET:H	1:C:309:ASN:HD21	1.49	0.61
1:A:103:GLU:OE2	1:A:251:ARG:NH2	2.29	0.60
1:A:247:PHE:O	1:A:251:ARG:HG3	2.00	0.60
1:B:297:ASP:OD1	1:B:299:GLU:HB2	2.01	0.60
1:A:151:ASP:OD1	1:A:152:GLU:N	2.31	0.60
1:C:140:LEU:O	1:C:144:THR:HG22	2.01	0.60
1:B:233:MET:H	1:B:309:ASN:HD21	1.50	0.60
1:D:324:HIS:CD2	1:D:327:GLN:OE1	2.50	0.60
1:A:309:ASN:HD22	1:A:309:ASN:H	1.49	0.60
1:A:136:THR:HG21	1:A:141:LEU:CB	2.32	0.60
1:C:294:TYR:HA	1:C:295:PRO:C	2.27	0.59
1:B:100:ILE:HG21	1:B:144:THR:HG21	1.84	0.59
1:B:169:ASN:ND2	1:B:172:LYS:HE2	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ILE:HG12	1:C:317:GLU:OE1	2.02	0.59
1:B:182:GLU:CD	1:B:182:GLU:H	2.10	0.59
1:C:112:ILE:HD11	1:C:126:ARG:HB3	1.84	0.58
1:C:136:THR:CG2	1:C:138:GLU:H	2.16	0.58
1:B:80:ASP:O	1:B:211:ILE:HD13	2.04	0.58
1:C:96:LEU:O	1:C:99:CYS:HB2	2.03	0.58
1:D:112:ILE:HD12	1:D:329:GLU:HB3	1.84	0.57
1:B:238:ASN:HD21	1:B:240:TYR:HB2	1.67	0.57
1:A:84:TYR:CE1	1:A:85:LEU:HG	2.38	0.57
1:D:108:GLY:HA2	1:D:327:GLN:NE2	2.18	0.57
1:C:224:VAL:O	1:C:228:LEU:HD23	2.04	0.57
1:D:288:MET:HE1	1:D:339:SER:CA	2.35	0.57
1:B:171:LEU:C	1:B:172:LYS:HG2	2.29	0.56
1:B:178:LYS:O	1:B:183:ARG:NH1	2.38	0.56
1:B:140:LEU:O	1:B:144:THR:HG23	2.04	0.56
1:B:294:TYR:CD1	1:B:295:PRO:HA	2.40	0.56
1:A:136:THR:HG22	1:A:142:ASP:CG	2.30	0.56
1:A:121:PHE:CE2	1:C:277:ARG:HD2	2.40	0.56
1:A:181:ARG:NH1	1:B:201:PHE:O	2.39	0.56
1:A:202:PHE:CD2	1:A:203:LEU:HD23	2.41	0.56
1:B:179:GLN:O	1:B:183:ARG:HD3	2.05	0.56
1:B:283:ARG:HE	1:B:307:SER:HB3	1.71	0.56
1:B:189:VAL:CG2	1:B:194:LEU:HD12	2.33	0.56
1:B:126:ARG:O	1:B:155:SER:HA	2.06	0.56
1:B:309:ASN:HD22	1:B:309:ASN:N	2.02	0.56
1:A:144:THR:HA	1:A:147:LEU:HD12	1.88	0.55
1:A:195:ARG:HG2	1:A:212:ALA:HB2	1.86	0.55
1:C:103:GLU:HG3	1:C:107:ARG:HE	1.70	0.55
1:D:309:ASN:H	1:D:309:ASN:ND2	1.98	0.55
1:B:100:ILE:HG23	1:B:141:LEU:HD23	1.89	0.55
1:C:123:LEU:HA	1:C:126:ARG:HD2	1.88	0.55
1:B:154:LEU:HB3	1:B:158:ASN:HD22	1.70	0.55
1:D:151:ASP:OD1	1:D:152:GLU:N	2.39	0.55
1:D:195:ARG:HG3	1:D:212:ALA:HB2	1.86	0.55
1:A:169:ASN:C	1:A:169:ASN:ND2	2.65	0.55
1:B:324:HIS:HD2	1:B:327:GLN:OE1	1.90	0.55
1:D:171:LEU:HD12	1:D:171:LEU:H	1.71	0.55
1:B:194:LEU:HB3	1:B:211:ILE:HA	1.89	0.55
1:B:124:SER:HB2	1:B:157:SER:HB2	1.89	0.55
1:B:161:ASP:HB3	1:B:167:THR:HG23	1.89	0.54
1:B:103:GLU:OE2	1:B:251:ARG:NH2	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LYS:O	1:C:183:ARG:NH1	2.40	0.54
1:C:202:PHE:CG	1:D:86:SER:HB2	2.43	0.54
1:B:233:MET:N	1:B:309:ASN:HD21	2.05	0.54
1:A:136:THR:N	1:A:142:ASP:OD1	2.36	0.54
1:B:82:GLU:OE1	1:B:82:GLU:HA	2.06	0.54
1:A:70:MET:HE2	1:A:70:MET:N	2.22	0.53
1:C:179:GLN:O	1:C:183:ARG:HB2	2.09	0.53
1:B:297:ASP:C	1:B:299:GLU:H	2.17	0.53
1:D:136:THR:OG1	1:D:142:ASP:OD2	2.25	0.53
1:B:67:LEU:HD21	1:B:193:VAL:HG21	1.90	0.53
1:B:101:ILE:O	1:B:102:ILE:C	2.48	0.53
1:C:136:THR:HG21	1:C:141:LEU:HB2	1.91	0.53
1:C:285:GLU:HA	1:C:288:MET:HB2	1.91	0.53
1:B:143:GLU:CD	1:B:183:ARG:NH2	2.67	0.53
1:C:309:ASN:HD22	1:C:309:ASN:N	2.03	0.53
1:D:154:LEU:HB3	1:D:158:ASN:ND2	2.24	0.53
1:D:178:LYS:O	1:D:183:ARG:NH1	2.41	0.53
1:D:194:LEU:HD12	1:D:211:ILE:HA	1.90	0.53
1:B:194:LEU:HA	1:B:212:ALA:N	2.23	0.53
1:A:150:ASN:O	1:A:150:ASN:CG	2.51	0.53
1:D:233:MET:N	1:D:309:ASN:HD21	2.03	0.53
1:A:169:ASN:C	1:A:169:ASN:HD22	2.17	0.52
1:D:158:ASN:O	1:D:162:LEU:HG	2.09	0.52
1:B:112:ILE:CD1	1:B:326:LEU:HD22	2.40	0.52
1:C:283:ARG:O	1:C:287:ILE:HG23	2.09	0.52
1:A:104:LEU:HB3	1:A:110:ILE:HG12	1.92	0.52
1:B:216:CYS:HB2	1:B:240:TYR:CE1	2.44	0.52
1:A:218:GLU:OE1	1:D:273:GLU:HA	2.09	0.52
1:A:196:THR:HB	1:A:209:HIS:CD2	2.44	0.51
1:A:198:MET:HE3	1:A:205:ASP:HB3	1.93	0.51
1:A:242:PRO:C	1:A:244:THR:H	2.18	0.51
1:A:321:ASN:ND2	1:A:324:HIS:CE1	2.79	0.51
1:C:172:LYS:HG2	1:C:175:TYR:OH	2.10	0.51
1:D:250:ILE:HG12	1:D:317:GLU:OE1	2.10	0.51
1:A:271:THR:HB	1:D:271:THR:HB	1.91	0.51
1:B:154:LEU:HD11	1:B:172:LYS:NZ	2.26	0.51
1:B:247:PHE:O	1:B:251:ARG:HG3	2.09	0.51
1:B:112:ILE:HD11	1:B:326:LEU:HD22	1.92	0.51
1:D:102:ILE:HG13	1:D:334:VAL:HG11	1.91	0.51
1:A:290:GLN:HB3	1:A:291:PHE:CD1	2.47	0.50
1:D:195:ARG:NH1	1:D:197:GLU:OE2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:NH1	1:A:81:ARG:O	2.44	0.50
1:B:144:THR:HG22	1:B:177:LEU:HD21	1.94	0.50
1:B:156:ILE:HG13	1:B:157:SER:N	2.26	0.50
1:D:96:LEU:O	1:D:99:CYS:HB2	2.12	0.50
1:D:111:ARG:HD3	1:D:131:ILE:HD11	1.93	0.50
1:B:106:LEU:CD1	1:B:331:ILE:CD1	2.89	0.50
1:B:247:PHE:HB3	1:B:250:ILE:HB	1.94	0.49
1:C:112:ILE:HD11	1:C:126:ARG:CB	2.42	0.49
1:B:68:THR:OG1	1:B:70:MET:HG2	2.13	0.49
1:C:169:ASN:ND2	1:C:172:LYS:H	2.10	0.49
1:B:132:ASP:OD1	1:B:133:SER:N	2.45	0.49
1:A:84:TYR:O	1:B:201:PHE:HB3	2.12	0.49
1:A:306:VAL:O	1:A:307:SER:C	2.55	0.49
1:D:148:MET:HG2	1:D:159:TRP:CZ2	2.48	0.49
1:B:249:ILE:HD11	1:B:314:VAL:HG22	1.93	0.49
1:B:247:PHE:HA	1:B:317:GLU:CD	2.38	0.49
1:C:169:ASN:CG	1:C:172:LYS:HB2	2.38	0.49
1:C:181:ARG:HD2	1:D:202:PHE:O	2.13	0.49
1:C:242:PRO:HD2	1:C:245:THR:CG2	2.43	0.49
1:A:140:LEU:O	1:A:144:THR:CG2	2.61	0.49
1:A:242:PRO:HD2	1:A:245:THR:HG23	1.89	0.49
1:C:288:MET:SD	1:C:339:SER:HB3	2.53	0.49
1:A:111:ARG:HD2	1:A:131:ILE:HG21	1.95	0.48
1:D:171:LEU:HD12	1:D:171:LEU:N	2.28	0.48
1:C:71:GLU:O	1:C:75:LEU:HD22	2.13	0.48
1:C:288:MET:HE1	1:C:335:PHE:O	2.13	0.48
1:B:249:ILE:HG23	1:B:317:GLU:OE2	2.13	0.48
1:D:101:ILE:CD1	1:D:334:VAL:CG2	2.89	0.48
1:B:181:ARG:HB2	1:B:182:GLU:OE2	2.14	0.48
1:C:259:SER:HB2	1:C:264:VAL:HG23	1.96	0.48
1:A:247:PHE:HB3	1:A:250:ILE:HB	1.95	0.47
1:C:136:THR:HG21	1:C:141:LEU:CB	2.44	0.47
1:B:242:PRO:O	1:B:245:THR:HG23	2.14	0.47
1:C:75:LEU:HD21	1:C:188:LEU:HD21	1.95	0.47
1:D:221:LYS:HG3	1:D:268:VAL:HG22	1.97	0.47
1:A:250:ILE:HG12	1:A:317:GLU:OE1	2.15	0.47
1:B:233:MET:H	1:B:309:ASN:ND2	2.11	0.47
1:A:86:SER:HB2	1:B:202:PHE:CG	2.49	0.47
1:D:255:LEU:O	1:D:255:LEU:HD22	2.15	0.46
1:A:182:GLU:OE2	1:A:182:GLU:N	2.45	0.46
1:D:316:GLU:O	1:D:320:ASN:ND2	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ARG:O	1:D:281:ILE:HG12	2.15	0.46
1:A:96:LEU:O	1:A:99:CYS:HB2	2.15	0.46
1:A:143:GLU:OE2	1:A:183:ARG:NH2	2.49	0.46
1:D:171:LEU:H	1:D:171:LEU:CD1	2.29	0.46
1:B:196:THR:HB	1:B:209:HIS:CD2	2.50	0.46
1:B:76:MET:HE3	1:B:76:MET:HB3	1.88	0.46
1:A:283:ARG:NH1	1:A:286:GLU:OE1	2.48	0.46
1:B:108:GLY:HA2	1:B:327:GLN:NE2	2.28	0.46
1:A:242:PRO:HD2	1:A:245:THR:HG22	1.91	0.46
1:C:84:TYR:CG	1:D:202:PHE:HB2	2.51	0.46
1:B:96:LEU:O	1:B:100:ILE:HG13	2.16	0.45
1:D:139:VAL:O	1:D:143:GLU:HG3	2.16	0.45
1:A:269:LEU:O	1:A:277:ARG:HD3	2.17	0.45
1:A:124:SER:HB3	1:A:336:GLU:OE1	2.16	0.45
1:D:103:GLU:HG2	1:D:141:LEU:HD11	1.97	0.45
1:D:310:LEU:O	1:D:314:VAL:HG23	2.16	0.45
1:B:196:THR:HB	1:B:209:HIS:HD2	1.80	0.45
1:B:237:TYR:CD1	1:B:237:TYR:N	2.85	0.45
1:B:324:HIS:CD2	1:B:327:GLN:OE1	2.70	0.45
1:C:147:LEU:HD22	1:C:175:TYR:CG	2.52	0.45
1:D:233:MET:HG2	1:D:235:LEU:HD13	1.99	0.45
1:C:136:THR:N	1:C:142:ASP:OD1	2.47	0.45
1:A:223:ARG:O	1:A:224:VAL:C	2.59	0.44
1:B:78:LEU:O	1:B:85:LEU:HD12	2.16	0.44
1:C:332:ALA:O	1:C:335:PHE:HB2	2.18	0.44
1:A:260:TYR:CD2	1:A:288:MET:HE3	2.52	0.44
1:B:138:GLU:HB2	1:B:141:LEU:HD12	2.00	0.44
1:C:247:PHE:O	1:C:251:ARG:HG3	2.17	0.44
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.76	0.44
1:A:321:ASN:ND2	1:A:324:HIS:HE1	2.16	0.44
1:C:171:LEU:O	1:C:173:ILE:N	2.49	0.44
1:D:288:MET:HE3	1:D:288:MET:HB3	1.77	0.44
1:A:242:PRO:C	1:A:244:THR:N	2.74	0.44
1:C:253:LEU:HD21	1:C:310:LEU:HD11	2.00	0.44
1:A:321:ASN:HD21	1:A:324:HIS:CE1	2.35	0.44
1:D:294:TYR:CD2	1:D:329:GLU:HG3	2.53	0.44
1:A:336:GLU:O	1:A:340:ARG:HG2	2.17	0.44
1:D:162:LEU:CD2	1:D:167:THR:HG21	2.47	0.44
1:C:97:ARG:HA	1:C:100:ILE:HD12	1.99	0.43
1:D:233:MET:HE2	1:D:233:MET:HB3	1.85	0.43
1:D:253:LEU:HD21	1:D:310:LEU:HD21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ARG:NH1	1:D:81:ARG:O	2.51	0.43
1:C:195:ARG:O	1:C:209:HIS:HA	2.19	0.43
1:A:70:MET:HG3	1:A:184:LEU:HD21	2.00	0.43
1:B:97:ARG:CG	1:B:164:SER:HB3	2.47	0.43
1:C:227:VAL:HG22	1:C:233:MET:HE2	2.01	0.43
1:A:221:LYS:HG3	1:A:268:VAL:HB	2.00	0.43
1:C:118:ARG:HB2	1:C:126:ARG:HG2	2.00	0.43
1:A:103:GLU:CG	1:A:141:LEU:HD11	2.48	0.43
1:A:136:THR:H	1:A:142:ASP:CG	2.26	0.43
1:D:342:ASP:OD1	1:D:342:ASP:N	2.41	0.43
1:A:88:TRP:CD2	1:A:181:ARG:HD3	2.54	0.43
1:B:143:GLU:CD	1:B:183:ARG:HH22	2.27	0.43
1:C:70:MET:HE3	1:C:70:MET:N	2.23	0.43
1:C:257:CYS:SG	1:C:288:MET:HG2	2.59	0.43
1:B:238:ASN:ND2	1:B:240:TYR:HB2	2.34	0.42
1:C:242:PRO:O	1:C:245:THR:HG23	2.19	0.42
1:A:143:GLU:CD	1:A:183:ARG:NH2	2.76	0.42
1:A:296:PHE:HE2	1:A:332:ALA:HB2	1.82	0.42
1:C:283:ARG:NH2	1:C:307:SER:HB3	2.34	0.42
1:B:148:MET:HG2	1:B:159:TRP:CZ2	2.54	0.42
1:A:109:LYS:HB3	1:A:145:LEU:HD11	2.01	0.42
1:A:132:ASP:OD1	1:A:132:ASP:C	2.63	0.42
1:C:109:LYS:HA	1:C:132:ASP:HB3	2.01	0.42
1:C:127:LEU:HA	1:C:155:SER:HA	2.02	0.42
1:A:294:TYR:HA	1:A:295:PRO:C	2.43	0.42
1:B:79:ARG:HB2	1:B:82:GLU:O	2.19	0.42
1:D:100:ILE:HG23	1:D:141:LEU:HD23	2.01	0.42
1:A:136:THR:HG22	1:A:142:ASP:OD2	2.19	0.42
1:B:112:ILE:HG13	1:B:326:LEU:O	2.20	0.42
1:B:154:LEU:HD11	1:B:172:LYS:HZ2	1.83	0.42
1:B:213:ASP:OD1	1:B:213:ASP:C	2.62	0.42
1:C:294:TYR:CG	1:C:295:PRO:HA	2.54	0.42
1:D:247:PHE:HA	1:D:317:GLU:OE1	2.20	0.42
1:A:111:ARG:HD2	1:A:131:ILE:CG2	2.49	0.42
1:B:101:ILE:C	1:B:103:GLU:N	2.78	0.42
1:B:288:MET:SD	1:B:339:SER:HB3	2.60	0.42
1:D:286:GLU:O	1:D:287:ILE:C	2.62	0.42
1:C:119:LYS:HA	1:C:126:ARG:NH2	2.35	0.41
1:C:130:VAL:HG21	1:C:149:LYS:HA	2.02	0.41
1:C:249:ILE:O	1:C:253:LEU:HG	2.20	0.41
1:C:248:LYS:O	1:C:252:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLN:OE1	1:A:297:ASP:HB2	2.21	0.41
1:A:296:PHE:CE2	1:A:332:ALA:HB2	2.55	0.41
1:A:152:GLU:O	1:A:154:LEU:HD13	2.20	0.41
1:B:182:GLU:CD	1:B:182:GLU:N	2.77	0.41
1:A:140:LEU:O	1:A:144:THR:HG22	2.20	0.41
1:A:166:GLU:OE1	1:A:166:GLU:HA	2.20	0.41
1:B:128:ILE:HD13	1:B:156:ILE:HG22	2.01	0.41
1:B:306:VAL:O	1:B:307:SER:HB3	2.21	0.41
1:D:73:VAL:HG12	1:D:96:LEU:HD21	2.02	0.41
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.85	0.41
1:C:331:ILE:HD12	1:C:335:PHE:CE2	2.55	0.41
1:D:233:MET:CG	1:D:235:LEU:HD13	2.51	0.41
1:B:72:GLU:O	1:B:76:MET:HG2	2.21	0.41
1:B:221:LYS:O	1:B:225:LEU:HB2	2.20	0.41
1:C:141:LEU:O	1:C:144:THR:HG23	2.21	0.41
1:C:338:PHE:O	1:C:341:MET:HG2	2.21	0.41
1:D:127:LEU:HA	1:D:155:SER:HA	2.02	0.41
1:C:182:GLU:O	1:C:185:ALA:HB3	2.21	0.41
1:C:104:LEU:HB3	1:C:110:ILE:HG12	2.03	0.40
1:D:213:ASP:OD1	1:D:213:ASP:C	2.64	0.40
1:C:125:GLU:OE1	1:C:125:GLU:HA	2.21	0.40
1:D:219:ALA:O	1:D:220:ILE:C	2.62	0.40
1:D:294:TYR:HA	1:D:295:PRO:C	2.47	0.40
1:D:309:ASN:HD22	1:D:309:ASN:N	1.94	0.40
1:A:237:TYR:CD1	1:A:237:TYR:N	2.90	0.40
1:C:311:ASN:O	1:C:312:LYS:C	2.64	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	279/288 (97%)	258 (92%)	21 (8%)	0	100	100
1	B	279/288 (97%)	250 (90%)	28 (10%)	1 (0%)	30	57
1	C	277/288 (96%)	253 (91%)	23 (8%)	1 (0%)	30	57
1	D	281/288 (98%)	256 (91%)	25 (9%)	0	100	100
All	All	1116/1152 (97%)	1017 (91%)	97 (9%)	2 (0%)	43	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	THR
1	C	173	ILE

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	226/260 (87%)	193 (85%)	33 (15%)	3	12
1	B	219/260 (84%)	183 (84%)	36 (16%)	2	9
1	C	221/260 (85%)	185 (84%)	36 (16%)	2	9
1	D	233/260 (90%)	195 (84%)	38 (16%)	2	9
All	All	899/1040 (86%)	756 (84%)	143 (16%)	2	10

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LEU
1	A	68	THR
1	A	70	MET
1	A	79	ARG
1	A	92	ILE
1	A	101	ILE
1	A	111	ARG
1	A	112	ILE
1	A	136	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	VAL
1	A	144	THR
1	A	150	ASN
1	A	152	GLU
1	A	167	THR
1	A	169	ASN
1	A	183	ARG
1	A	195	ARG
1	A	196	THR
1	A	203	LEU
1	A	211	ILE
1	A	226	SER
1	A	228	LEU
1	A	229	VAL
1	A	244	THR
1	A	275	GLU
1	A	282	SER
1	A	293	GLN
1	A	308	VAL
1	A	309	ASN
1	A	310	LEU
1	A	325	ASP
1	A	327	GLN
1	A	340	ARG
1	B	66	THR
1	B	70	MET
1	B	78	LEU
1	B	85	LEU
1	B	92	ILE
1	B	106	LEU
1	B	112	ILE
1	B	116	SER
1	B	125	GLU
1	B	128	ILE
1	B	132	ASP
1	B	134	SER
1	B	139	VAL
1	B	144	THR
1	B	145	LEU
1	B	156	ILE
1	B	175	TYR
1	B	181	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	182	GLU
1	B	189	VAL
1	B	194	LEU
1	B	196	THR
1	B	211	ILE
1	B	217	LYS
1	B	225	LEU
1	B	227	VAL
1	B	232	ASN
1	B	246	SER
1	B	249	ILE
1	B	272	LEU
1	B	281	ILE
1	B	293	GLN
1	B	309	ASN
1	B	310	LEU
1	B	313	GLU
1	B	326	LEU
1	C	70	MET
1	C	74	LEU
1	C	75	LEU
1	C	91	SER
1	C	101	ILE
1	C	106	LEU
1	C	111	ARG
1	C	128	ILE
1	C	129	GLU
1	C	131	ILE
1	C	136	THR
1	C	139	VAL
1	C	144	THR
1	C	145	LEU
1	C	166	GLU
1	C	169	ASN
1	C	170	LEU
1	C	181	ARG
1	C	183	ARG
1	C	194	LEU
1	C	208	THR
1	C	211	ILE
1	C	228	LEU
1	C	252	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	265	LEU
1	C	266	GLU
1	C	273	GLU
1	C	285	GLU
1	C	287	ILE
1	C	288	MET
1	C	290	GLN
1	C	306	VAL
1	C	307	SER
1	C	308	VAL
1	C	309	ASN
1	C	331	ILE
1	D	73	VAL
1	D	75	LEU
1	D	81	ARG
1	D	101	ILE
1	D	112	ILE
1	D	119	LYS
1	D	120	ARG
1	D	139	VAL
1	D	144	THR
1	D	145	LEU
1	D	147	LEU
1	D	154	LEU
1	D	166	GLU
1	D	167	THR
1	D	169	ASN
1	D	170	LEU
1	D	171	LEU
1	D	174	ASN
1	D	182	GLU
1	D	183	ARG
1	D	194	LEU
1	D	208	THR
1	D	228	LEU
1	D	229	VAL
1	D	231	ARG
1	D	232	ASN
1	D	236	SER
1	D	255	LEU
1	D	268	VAL
1	D	279	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	288	MET
1	D	293	GLN
1	D	302	THR
1	D	308	VAL
1	D	309	ASN
1	D	310	LEU
1	D	342	ASP
1	D	343	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	209	HIS
1	A	309	ASN
1	A	321	ASN
1	A	324	HIS
1	B	158	ASN
1	B	169	ASN
1	B	176	GLN
1	B	209	HIS
1	B	267	ASN
1	B	290	GLN
1	B	293	GLN
1	B	309	ASN
1	B	320	ASN
1	B	324	HIS
1	B	327	GLN
1	C	146	GLN
1	C	158	ASN
1	C	169	ASN
1	C	176	GLN
1	C	290	GLN
1	C	309	ASN
1	C	320	ASN
1	C	324	HIS
1	D	63	ASN
1	D	146	GLN
1	D	158	ASN
1	D	174	ASN
1	D	176	GLN
1	D	232	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	309	ASN
1	D	324	HIS

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	281/288 (97%)	-0.16	3 (1%) 78 57	25, 38, 53, 68	0
1	B	281/288 (97%)	0.13	5 (1%) 67 45	32, 49, 65, 70	0
1	C	279/288 (96%)	0.04	7 (2%) 58 35	31, 46, 63, 66	0
1	D	283/288 (98%)	-0.12	3 (1%) 78 57	22, 40, 56, 66	0
All	All	1124/1152 (97%)	-0.03	18 (1%) 70 47	22, 44, 62, 70	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	SER	3.1
1	C	307	SER	2.9
1	C	303	GLU	2.6
1	D	168	TRP	2.6
1	C	173	ILE	2.6
1	B	342	ASP	2.5
1	C	301	GLU	2.4
1	C	175	TYR	2.4
1	A	200	ASN	2.3
1	D	200	ASN	2.3
1	D	90	ASP	2.3
1	B	85	LEU	2.2
1	B	248	LYS	2.1
1	A	343	MET	2.1
1	C	167	THR	2.1
1	B	117	ALA	2.1
1	A	201	PHE	2.0
1	B	62	ILE	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.