



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:22 AM UTC

PDB ID : 1AOW / pdb_00001aow
Title : ANNEXIN IV
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Deposited on : 1997-07-11
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

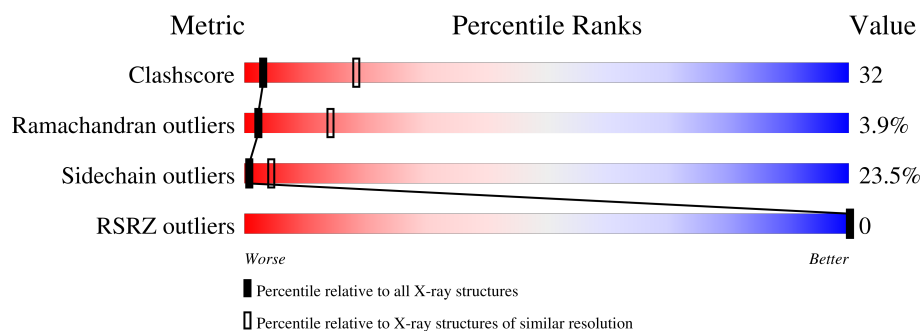
1 Overall quality at a glance

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))
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	309	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2448 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 ANNEXIN IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2448	1520	428	485	15			

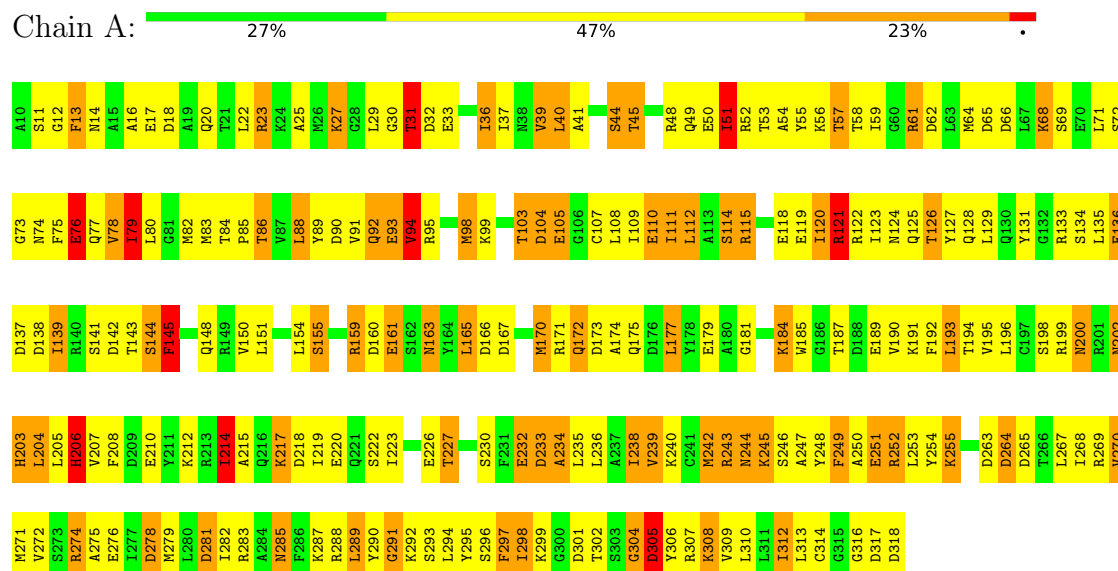
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	VAL	LEU	conflict	UNP P13214

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: ANNEXIN IV



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	118.56Å 118.56Å 82.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.0 (15.00-3.00) 94.4 (15.00-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.98Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.190 , 0.269 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.29 , 489.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2448	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.18	10/2476 (0.4%)	2.19	98/3320 (3.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	79	ILE	CA-CB	6.68	1.63	1.54
1	A	31	THR	CA-CB	6.64	1.64	1.53
1	A	206	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	139	ILE	CA-CB	5.93	1.62	1.54
1	A	203	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	57	THR	CA-CB	5.55	1.62	1.53
1	A	94	VAL	CA-CB	5.37	1.61	1.54
1	A	93	GLU	CA-C	-5.10	1.46	1.52
1	A	145	PHE	CA-CB	5.08	1.62	1.53
1	A	111	ILE	CA-CB	5.06	1.61	1.54

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	ASP	CA-CB-CG	13.03	125.63	112.60
1	A	318	ASP	CA-CB-CG	11.33	123.93	112.60
1	A	317	ASP	O-C-N	11.18	135.96	123.10
1	A	278	ASP	CA-CB-CG	10.41	123.01	112.60
1	A	76	GLU	N-CA-C	-9.74	98.22	111.96
1	A	124	ASN	OD1-CG-ND2	-9.28	113.32	122.60
1	A	104	ASP	CA-CB-CG	9.21	121.81	112.60
1	A	134	SER	N-CA-C	9.08	122.51	110.53
1	A	18	ASP	CA-CB-CG	8.86	121.46	112.60
1	A	145	PHE	CA-CB-CG	8.68	122.47	113.80
1	A	235	LEU	N-CA-C	-8.51	101.97	111.07
1	A	238	ILE	CA-C-O	-8.36	112.31	121.17
1	A	78	VAL	N-CA-C	8.14	118.19	110.53
1	A	265	ASP	CA-CB-CG	7.79	120.39	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	THR	O-C-N	7.73	130.03	122.07
1	A	202	ASN	OD1-CG-ND2	-7.70	114.90	122.60
1	A	93	GLU	CA-C-O	-7.62	113.05	120.90
1	A	163	ASN	CA-CB-CG	7.54	120.14	112.60
1	A	124	ASN	CA-CB-CG	-7.53	105.07	112.60
1	A	285	ASN	OD1-CG-ND2	-7.32	115.28	122.60
1	A	270	VAL	CB-CA-C	-7.27	102.72	111.81
1	A	200	ASN	OD1-CG-ND2	-7.24	115.36	122.60
1	A	92	GLN	OE1-CD-NE2	-7.20	115.40	122.60
1	A	249	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	14	ASN	OD1-CG-ND2	-7.06	115.54	122.60
1	A	103	THR	N-CA-CB	-7.06	101.76	112.28
1	A	238	ILE	N-CA-C	-7.00	103.70	110.42
1	A	270	VAL	N-CA-CB	6.98	118.23	110.62
1	A	317	ASP	CA-C-N	6.92	134.16	121.70
1	A	317	ASP	C-N-CA	6.92	134.16	121.70
1	A	214	ILE	CB-CG1-CD1	6.90	128.29	113.80
1	A	105	GLU	CA-C-N	6.80	127.53	119.98
1	A	105	GLU	C-N-CA	6.80	127.53	119.98
1	A	93	GLU	O-C-N	6.68	129.25	122.03
1	A	305	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	142	ASP	N-CA-C	6.60	120.79	112.87
1	A	98	MET	N-CA-C	6.59	124.85	110.80
1	A	128	GLN	N-CA-C	-6.49	102.86	111.24
1	A	276	GLU	CA-CB-CG	-6.45	101.20	114.10
1	A	74	ASN	O-C-N	6.43	129.53	122.20
1	A	138	ASP	CA-C-N	6.29	129.35	120.42
1	A	138	ASP	C-N-CA	6.29	129.35	120.42
1	A	77	GLN	OE1-CD-NE2	-6.25	116.36	122.60
1	A	119	GLU	N-CA-C	-6.17	104.18	111.03
1	A	143	THR	N-CA-C	-6.14	99.80	109.50
1	A	239	VAL	N-CA-C	6.09	117.57	110.62
1	A	244	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	89	TYR	N-CA-C	-6.03	104.78	111.36
1	A	264	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	79	ILE	N-CA-C	-6.00	104.66	110.72
1	A	233	ASP	CB-CA-C	-6.00	101.22	110.81
1	A	268	ILE	N-CA-CB	-5.99	104.10	110.62
1	A	163	ASN	OD1-CG-ND2	-5.94	116.66	122.60
1	A	145	PHE	CA-C-N	5.92	128.68	120.63
1	A	145	PHE	C-N-CA	5.92	128.68	120.63
1	A	57	THR	N-CA-CB	-5.88	101.47	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ALA	N-CA-C	5.80	117.68	111.36
1	A	227	THR	N-CA-CB	-5.76	101.97	110.85
1	A	121	ARG	N-CA-C	5.73	117.99	111.11
1	A	239	VAL	N-CA-CB	-5.73	103.31	110.47
1	A	45	THR	CA-CB-OG1	-5.72	101.01	109.60
1	A	220	GLU	O-C-N	5.72	128.21	122.03
1	A	243	ARG	N-CA-C	-5.72	104.46	112.12
1	A	232	GLU	CA-C-O	-5.70	114.81	120.90
1	A	119	GLU	CA-C-O	-5.69	115.04	120.90
1	A	94	VAL	N-CA-CB	5.66	118.23	110.54
1	A	23	ARG	N-CA-C	5.61	117.25	111.03
1	A	74	ASN	N-CA-C	5.59	118.91	111.75
1	A	51	ILE	N-CA-C	-5.57	104.94	110.62
1	A	20	GLN	CB-CG-CD	5.57	122.07	112.60
1	A	20	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	A	263	ASP	CB-CA-C	5.43	120.30	112.05
1	A	308	LYS	CG-CD-CE	5.39	123.69	111.30
1	A	254	TYR	O-C-N	5.37	127.68	122.09
1	A	297	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	39	VAL	CB-CA-C	-5.35	102.52	111.29
1	A	120	ILE	CB-CA-C	-5.33	105.06	111.88
1	A	39	VAL	N-CA-CB	5.29	119.96	111.23
1	A	206	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	202	ASN	CB-CA-C	-5.25	102.61	110.90
1	A	281	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	16	ALA	N-CA-C	5.24	117.40	111.11
1	A	177	LEU	CD1-CG-CD2	-5.23	99.30	110.80
1	A	172	GLN	OE1-CD-NE2	-5.21	117.39	122.60
1	A	94	VAL	CG1-CB-CG2	-5.20	99.35	110.80
1	A	30	GLY	CA-C-O	-5.17	111.56	120.57
1	A	72	SER	O-C-N	5.17	128.75	122.85
1	A	263	ASP	N-CA-CB	-5.14	102.93	110.49
1	A	276	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	57	THR	CB-CA-C	5.10	119.52	110.85
1	A	88	LEU	N-CA-C	-5.09	105.82	112.23
1	A	111	ILE	CA-C-N	-5.08	114.54	122.42
1	A	111	ILE	C-N-CA	-5.08	114.54	122.42
1	A	297	PHE	N-CA-C	-5.08	105.64	111.07
1	A	163	ASN	CB-CG-ND2	5.06	123.99	116.40
1	A	312	ILE	O-C-N	-5.05	116.25	122.57
1	A	161	GLU	CB-CG-CD	5.03	121.14	112.60
1	A	202	ASN	N-CA-CB	5.02	117.35	110.07

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	2448	0	2439	154	0
All	All	2448	0	2439	154	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 32.

All (154) 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:A:165:LEU:HD23	1:A:203:HIS:HA	1.48	0.96
1:A:194:THR:HG22	1:A:199:ARG:HH12	1.33	0.93
1:A:165:LEU:HD21	1:A:170:MET:HG3	1.56	0.87
1:A:114:SER:HB2	1:A:115:ARG:HH11	1.38	0.87
1:A:94:VAL:HG22	1:A:111:ILE:HG21	1.58	0.84
1:A:78:VAL:HG11	1:A:306:TYR:HE1	1.46	0.80
1:A:194:THR:HG22	1:A:199:ARG:NH1	2.01	0.75
1:A:114:SER:HB2	1:A:115:ARG:NH1	2.04	0.73
1:A:305:ASP:HA	1:A:308:LYS:HB2	1.71	0.72
1:A:88:LEU:HG	1:A:92:GLN:OE1	1.90	0.71
1:A:250:ALA:HA	1:A:253:LEU:HD12	1.73	0.70
1:A:165:LEU:HG	1:A:206:HIS:CD2	2.26	0.70
1:A:177:LEU:HD11	1:A:195:VAL:HG11	1.74	0.69
1:A:150:VAL:HA	1:A:193:LEU:HD11	1.75	0.69
1:A:253:LEU:HD13	1:A:294:LEU:HD13	1.75	0.68
1:A:22:LEU:HD21	1:A:40:LEU:HD23	1.76	0.68
1:A:163:ASN:OD1	1:A:202:ASN:HB2	1.94	0.68
1:A:251:GLU:O	1:A:255:LYS:HB2	1.93	0.67
1:A:90:ASP:O	1:A:94:VAL:HG23	1.94	0.67
1:A:309:VAL:HA	1:A:312:ILE:HD12	1.78	0.66
1:A:222:SER:HB3	1:A:226:GLU:OE2	1.95	0.66
1:A:110:GLU:HG3	1:A:252:ARG:HD3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ALA:HB1	1:A:32:ASP:HB3	1.78	0.65
1:A:294:LEU:HG	1:A:298:ILE:HD11	1.78	0.65
1:A:91:VAL:HG22	1:A:123:ILE:HG23	1.78	0.65
1:A:249:PHE:O	1:A:253:LEU:HG	1.97	0.64
1:A:287:LYS:HA	1:A:292:LYS:O	1.98	0.64
1:A:223:ILE:O	1:A:227:THR:HB	1.97	0.64
1:A:299:LYS:HA	1:A:307:ARG:HD3	1.80	0.64
1:A:165:LEU:CD2	1:A:203:HIS:HA	2.25	0.64
1:A:227:THR:HG22	1:A:232:GLU:HB2	1.81	0.63
1:A:279:MET:HA	1:A:282:ILE:HD12	1.81	0.62
1:A:283:ARG:HD2	1:A:314:CYS:SG	2.39	0.62
1:A:48:ARG:O	1:A:51:ILE:HB	1.99	0.62
1:A:236:LEU:O	1:A:240:LYS:HG2	1.99	0.62
1:A:234:ALA:O	1:A:238:ILE:HG13	1.99	0.61
1:A:49:GLN:O	1:A:52:ARG:HB2	2.02	0.60
1:A:62:ASP:HB3	1:A:65:ASP:OD2	2.02	0.59
1:A:189:GLU:HA	1:A:192:PHE:CE1	2.37	0.59
1:A:135:LEU:HD23	1:A:155:SER:HB2	1.84	0.59
1:A:244:ASN:ND2	1:A:247:ALA:HB2	2.18	0.58
1:A:41:ALA:HA	1:A:48:ARG:HH21	1.68	0.58
1:A:304:GLY:O	1:A:308:LYS:HG3	2.04	0.58
1:A:181:GLY:HA2	1:A:185:TRP:HE1	1.68	0.58
1:A:40:LEU:HD11	1:A:83:MET:HG2	1.86	0.58
1:A:41:ALA:HA	1:A:48:ARG:NH2	2.19	0.58
1:A:33:GLU:HA	1:A:36:ILE:HD13	1.87	0.57
1:A:240:LYS:HB3	1:A:248:TYR:HB2	1.87	0.57
1:A:275:ALA:HB2	1:A:313:LEU:HD13	1.87	0.56
1:A:172:GLN:O	1:A:175:GLN:HB3	2.05	0.56
1:A:271:MET:O	1:A:275:ALA:HB2	2.06	0.56
1:A:181:GLY:HA2	1:A:185:TRP:NE1	2.21	0.56
1:A:144:SER:HB2	1:A:145:PHE:CD1	2.42	0.55
1:A:165:LEU:HD11	1:A:170:MET:SD	2.46	0.55
1:A:278:ASP:HB2	1:A:281:ASP:HB2	1.88	0.55
1:A:189:GLU:HA	1:A:192:PHE:CZ	2.43	0.54
1:A:293:SER:OG	1:A:295:TYR:HB3	2.06	0.54
1:A:244:ASN:HD21	1:A:285:ASN:ND2	2.06	0.54
1:A:75:PHE:HA	1:A:78:VAL:HG22	1.90	0.54
1:A:121:ARG:HB3	1:A:121:ARG:NH1	2.23	0.54
1:A:23:ARG:NH2	1:A:27:LYS:HG2	2.23	0.53
1:A:79:ILE:HD13	1:A:82:MET:HE2	1.90	0.53
1:A:296:SER:HA	1:A:299:LYS:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LEU:O	1:A:208:PHE:HB2	2.07	0.53
1:A:112:LEU:HD23	1:A:154:LEU:HB2	1.92	0.52
1:A:159:ARG:HG2	1:A:198:SER:HA	1.91	0.52
1:A:245:LYS:O	1:A:249:PHE:HD2	1.93	0.52
1:A:44:SER:O	1:A:48:ARG:HG3	2.08	0.52
1:A:66:ASP:HA	1:A:69:SER:HG	1.75	0.52
1:A:302:THR:OG1	1:A:307:ARG:HG3	2.10	0.51
1:A:174:ALA:HB3	1:A:210:GLU:HG3	1.93	0.51
1:A:66:ASP:HA	1:A:69:SER:OG	2.10	0.51
1:A:64:MET:SD	1:A:83:MET:HB3	2.51	0.50
1:A:248:TYR:O	1:A:252:ARG:HG2	2.11	0.50
1:A:305:ASP:O	1:A:309:VAL:HG12	2.11	0.50
1:A:91:VAL:HG21	1:A:126:THR:HB	1.94	0.48
1:A:109:ILE:HG12	1:A:234:ALA:HB2	1.94	0.48
1:A:49:GLN:OE1	1:A:85:PRO:HD3	2.13	0.48
1:A:133:ARG:N	1:A:133:ARG:HD3	2.29	0.48
1:A:204:LEU:HD12	1:A:242:MET:SD	2.54	0.48
1:A:33:GLU:O	1:A:37:ILE:HD12	2.15	0.47
1:A:91:VAL:HG21	1:A:126:THR:CB	2.44	0.47
1:A:45:THR:O	1:A:48:ARG:HB2	2.14	0.47
1:A:166:ASP:O	1:A:170:MET:HB3	2.15	0.47
1:A:227:THR:HG22	1:A:232:GLU:CB	2.44	0.47
1:A:278:ASP:O	1:A:282:ILE:HG13	2.13	0.47
1:A:68:LYS:HD3	1:A:80:LEU:HD11	1.96	0.47
1:A:308:LYS:O	1:A:312:ILE:HG13	2.14	0.47
1:A:301:ASP:O	1:A:302:THR:HG23	2.15	0.47
1:A:136:GLU:HA	1:A:139:ILE:HD12	1.97	0.47
1:A:173:ASP:O	1:A:177:LEU:HD12	2.15	0.47
1:A:194:THR:HA	1:A:198:SER:OG	2.15	0.47
1:A:247:ALA:O	1:A:251:GLU:HB2	2.15	0.47
1:A:289:LEU:HD22	1:A:290:TYR:CZ	2.49	0.47
1:A:127:TYR:HA	1:A:131:TYR:HE2	1.80	0.46
1:A:287:LYS:O	1:A:291:GLY:HA2	2.15	0.46
1:A:111:ILE:HD11	1:A:269:ARG:HD2	1.97	0.46
1:A:175:GLN:HE21	1:A:175:GLN:HA	1.81	0.46
1:A:95:ARG:HG2	1:A:131:TYR:CE1	2.50	0.46
1:A:23:ARG:CZ	1:A:27:LYS:HG2	2.46	0.46
1:A:61:ARG:HG2	1:A:61:ARG:HH11	1.80	0.46
1:A:112:LEU:HD23	1:A:154:LEU:CB	2.45	0.46
1:A:159:ARG:HH21	1:A:242:MET:HE3	1.81	0.46
1:A:274:ARG:HD2	1:A:274:ARG:HA	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LYS:HD3	1:A:218:ASP:HB2	1.96	0.45
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.86	0.45
1:A:181:GLY:HA2	1:A:185:TRP:CD1	2.51	0.45
1:A:215:ALA:C	1:A:217:LYS:H	2.25	0.45
1:A:203:HIS:O	1:A:207:VAL:HG23	2.17	0.45
1:A:279:MET:HG2	1:A:313:LEU:O	2.16	0.45
1:A:107:CYS:SG	1:A:111:ILE:HG13	2.57	0.45
1:A:167:ASP:HB3	1:A:171:ARG:HH12	1.82	0.45
1:A:167:ASP:O	1:A:171:ARG:HB2	2.16	0.45
1:A:249:PHE:HD1	1:A:270:VAL:HG13	1.82	0.45
1:A:127:TYR:HA	1:A:131:TYR:CE2	2.52	0.45
1:A:200:ASN:OD1	1:A:202:ASN:HB3	2.17	0.45
1:A:109:ILE:HD13	1:A:233:ASP:HB3	2.00	0.44
1:A:136:GLU:HA	1:A:139:ILE:HB	1.99	0.44
1:A:184:LYS:O	1:A:185:TRP:HB2	2.17	0.44
1:A:205:LEU:HA	1:A:208:PHE:HB2	1.98	0.44
1:A:295:TYR:HB2	1:A:316:GLY:O	2.17	0.44
1:A:75:PHE:O	1:A:79:ILE:HB	2.17	0.44
1:A:93:GLU:OE1	1:A:93:GLU:HA	2.17	0.44
1:A:239:VAL:O	1:A:243:ARG:HB2	2.17	0.44
1:A:136:GLU:HG3	1:A:137:ASP:N	2.30	0.44
1:A:150:VAL:HA	1:A:193:LEU:CD1	2.47	0.44
1:A:76:GLU:O	1:A:80:LEU:HB2	2.18	0.43
1:A:103:THR:O	1:A:104:ASP:C	2.61	0.43
1:A:148:GLN:O	1:A:151:LEU:HB2	2.18	0.43
1:A:192:PHE:CE2	1:A:193:LEU:HD23	2.53	0.43
1:A:115:ARG:NH2	1:A:274:ARG:HH11	2.16	0.43
1:A:71:LEU:HD22	1:A:75:PHE:HD2	1.83	0.43
1:A:91:VAL:CG2	1:A:123:ILE:HG23	2.48	0.43
1:A:210:GLU:OE1	1:A:214:ILE:HG13	2.18	0.43
1:A:230:SER:O	1:A:233:ASP:HB2	2.18	0.42
1:A:31:THR:HG22	1:A:32:ASP:N	2.35	0.42
1:A:54:ALA:O	1:A:56:LYS:N	2.53	0.42
1:A:78:VAL:HG11	1:A:306:TYR:CE1	2.37	0.42
1:A:40:LEU:HD21	1:A:83:MET:SD	2.60	0.42
1:A:13:PHE:HZ	1:A:50:GLU:HB3	1.85	0.42
1:A:294:LEU:O	1:A:298:ILE:HG13	2.20	0.42
1:A:295:TYR:CE1	1:A:299:LYS:HD3	2.54	0.42
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.82	0.42
1:A:58:THR:O	1:A:59:ILE:HD13	2.20	0.41
1:A:223:ILE:HG21	1:A:236:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:THR:HB	1:A:105:GLU:HG3	2.01	0.41
1:A:110:GLU:OE1	1:A:270:VAL:HG22	2.20	0.41
1:A:93:GLU:OE2	1:A:269:ARG:HD3	2.20	0.41
1:A:210:GLU:CD	1:A:214:ILE:HG13	2.46	0.41
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.91	0.41
1:A:84:THR:HG23	1:A:85:PRO:HD2	2.03	0.41
1:A:267:LEU:HG	1:A:271:MET:HG2	2.02	0.40
1:A:95:ARG:HA	1:A:127:TYR:HE1	1.86	0.40
1:A:13:PHE:CZ	1:A:50:GLU:HB3	2.57	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	307/309 (99%)	241 (78%)	54 (18%)	12 (4%)	2 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	98	MET
1	A	39	VAL
1	A	73	GLY
1	A	304	GLY
1	A	55	TYR
1	A	99	LYS
1	A	264	ASP
1	A	291	GLY
1	A	86	THR
1	A	12	GLY
1	A	190	VAL

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	264/264 (100%)	202 (76%)	62 (24%)	1 4

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	13	PHE
1	A	17	GLU
1	A	27	LYS
1	A	29	LEU
1	A	36	ILE
1	A	40	LEU
1	A	44	SER
1	A	51	ILE
1	A	57	THR
1	A	61	ARG
1	A	68	LYS
1	A	76	GLU
1	A	79	ILE
1	A	86	THR
1	A	94	VAL
1	A	108	LEU
1	A	110	GLU
1	A	112	LEU
1	A	114	SER
1	A	115	ARG
1	A	118	GLU
1	A	120	ILE
1	A	121	ARG
1	A	122	ARG
1	A	125	GLN
1	A	126	THR
1	A	129	LEU
1	A	136	GLU
1	A	141	SER

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Mol	Chain	Res	Type
1	A	144	SER
1	A	145	PHE
1	A	155	SER
1	A	159	ARG
1	A	161	GLU
1	A	165	LEU
1	A	170	MET
1	A	179	GLU
1	A	184	LYS
1	A	187	THR
1	A	191	LYS
1	A	193	LEU
1	A	196	LEU
1	A	204	LEU
1	A	206	HIS
1	A	214	ILE
1	A	217	LYS
1	A	219	ILE
1	A	242	MET
1	A	245	LYS
1	A	246	SER
1	A	251	GLU
1	A	252	ARG
1	A	255	LYS
1	A	272	VAL
1	A	274	ARG
1	A	288	ARG
1	A	289	LEU
1	A	297	PHE
1	A	298	ILE
1	A	305	ASP
1	A	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	124	ASN
1	A	172	GLN
1	A	175	GLN
1	A	244	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	309/309 (100%)	-1.90	0	100 100	2, 17, 55, 109	0

There are no RSRZ outliers to report.

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.