



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 06:51 am BST

PDB ID : 1AOW
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

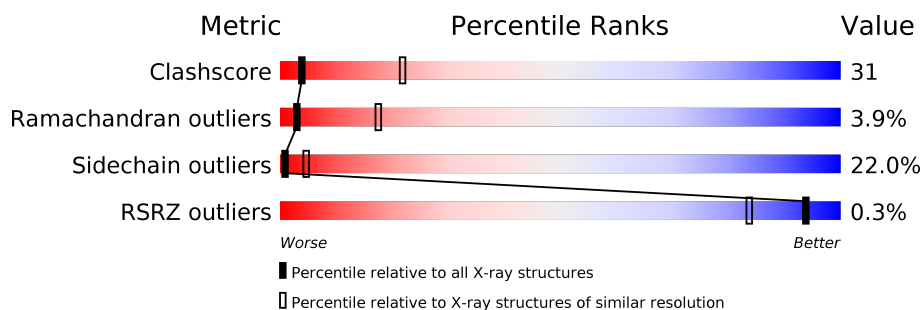
1 Overall quality at a glance

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on 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			

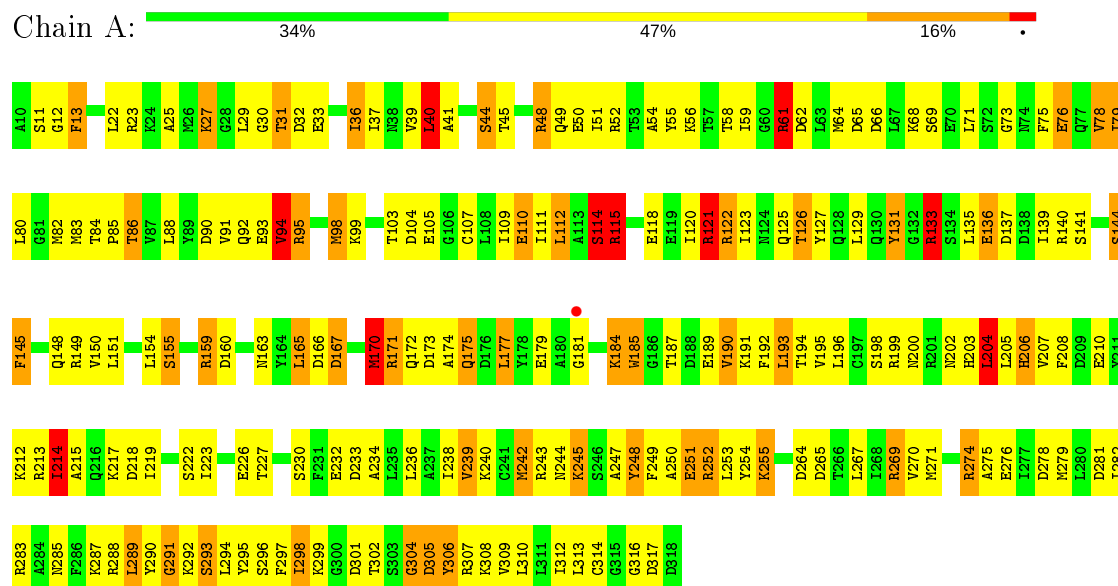
There is a discrepancy between the modelled and reference sequences:

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

3 Residue-property plots [i](#)

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: ANNEXIN IV



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	118.56 Å 118.56 Å 82.23 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 12.55 – 2.99	Depositor EDS
% Data completeness (in resolution range)	95.0 (15.00-3.00) 94.3 (12.55-2.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.98 Å)	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)	0.82 , 355.3	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	0.81	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

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	0.90	0/2476	1.78	44/3320 (1.3%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	61	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	133	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	248	TYR	CB-CG-CD2	-8.71	115.78	121.00
1	A	121	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	133	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	317	ASP	O-C-N	8.29	135.96	122.70
1	A	149	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	A	104	ASP	CB-CG-OD1	7.60	125.14	118.30
1	A	185	TRP	CD1-CG-CD2	7.56	112.35	106.30
1	A	171	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	317	ASP	CB-CG-OD1	7.51	125.06	118.30
1	A	94	VAL	CG1-CB-CG2	-7.22	99.35	110.90
1	A	122	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	171	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	185	TRP	CE2-CD2-CG	-6.86	101.81	107.30
1	A	317	ASP	CA-C-N	-6.66	102.55	117.20
1	A	40	LEU	CA-CB-CG	6.62	130.51	115.30
1	A	48	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	265	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	190	VAL	CG1-CB-CG2	-6.25	100.89	110.90
1	A	269	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	A	254	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	A	131	TYR	CB-CG-CD2	-6.10	117.34	121.00
1	A	204	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	140	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	170	MET	CG-SD-CE	-5.84	90.85	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	78	VAL	CA-CB-CG1	-5.66	102.41	110.90
1	A	213	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	160	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	239	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	A	160	ASP	CA-CB-CG	5.56	125.63	113.40
1	A	276	GLU	CA-CB-CG	-5.54	101.20	113.40
1	A	115	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	269	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	78	VAL	CG1-CB-CG2	5.17	119.17	110.90
1	A	214	ILE	CB-CG1-CD1	5.14	128.29	113.90
1	A	98	MET	N-CA-C	5.13	124.85	111.00
1	A	170	MET	CA-CB-CG	5.11	121.98	113.30
1	A	114	SER	N-CA-CB	-5.05	102.92	110.50
1	A	30	GLY	CA-C-O	-5.02	111.56	120.60
1	A	248	TYR	CD1-CG-CD2	5.01	123.41	117.90
1	A	306	TYR	CB-CG-CD2	-5.01	118.00	121.00

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	150	0
All	All	2448	0	2439	150	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 31.

All (150) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:240:LYS:HB3	1:A:248:TYR:HB2	1.87	0.57
1:A:33:GLU:HA	1:A:36:ILE:HD13	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:121:ARG:NH1	1:A:121:ARG:HB3	2.23	0.54
1:A:75:PHE:HA	1:A:78:VAL:HG22	1.90	0.54
1:A:23:ARG:NH2	1:A:27:LYS:HG2	2.23	0.53
1:A:296:SER:HA	1:A:299:LYS:HB2	1.91	0.53
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: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:248:TYR:O	1:A:252:ARG:HG2	2.11	0.50
1:A:64:MET:SD	1:A:83:MET:HB3	2.51	0.50
1:A:305:ASP:O	1:A:309:VAL:HG12	2.11	0.50
1:A:109:ILE:HG12	1:A:234:ALA:HB2	1.94	0.48
1:A:91:VAL:HG21	1:A:126:THR:HB	1.94	0.48
1:A:133:ARG:HD3	1:A:133:ARG:N	2.29	0.48
1:A:49:GLN:OE1	1:A:85:PRO:HD3	2.13	0.48
1:A:204:LEU:HD12	1:A:242:MET:SD	2.54	0.48
1:A:91:VAL:HG21	1:A:126:THR:CB	2.44	0.47
1:A:33:GLU:O	1:A:37:ILE:HD12	2.15	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:45:THR:O	1:A:48:ARG:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:175:GLN:HE21	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:HH11	1:A:61:ARG:HG2	1.80	0.46
1:A:112:LEU:HD23	1:A:154:LEU:CB	2.45	0.46
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.67	0.46
1:A:212:LYS:HD3	1:A:218:ASP:HB2	1.96	0.45
1:A:181:GLY:HA2	1:A:185:TRP:CD1	2.51	0.45
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.86	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:239:VAL:O	1:A:243:ARG:HB2	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: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:148:GLN:O	1:A:151:LEU:HB2	2.18	0.43
1:A:76:GLU:O	1:A:80:LEU:HB2	2.18	0.43
1:A:192:PHE:CE2	1:A:193:LEU:HD23	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ARG:NH2	1:A:274:ARG:HH11	2.16	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:71:LEU:HD22	1:A:75:PHE:HD2	1.83	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:79:ILE:HD13	1:A:82:MET:HE2	2.02	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:HA	1:A:313:LEU:HD23	1.82	0.42
1:A:223:ILE:HG21	1:A:236:LEU:HD13	2.02	0.41
1:A:58:THR:O	1:A:59:ILE:HD13	2.20	0.41
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:71:LEU:HA	1:A:71:LEU:HD23	1.91	0.41
1:A:84:THR:HG23	1:A:85:PRO:HD2	2.03	0.41
1:A:215:ALA:C	1:A:217:LYS:H	2.25	0.40
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 ⓘ

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	307/309 (99%)	241 (78%)	54 (18%)	12 (4%)	3 17

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%)	206 (78%)	58 (22%)	1 4

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	13	PHE
1	A	27	LYS
1	A	29	LEU
1	A	36	ILE
1	A	40	LEU
1	A	44	SER
1	A	61	ARG
1	A	76	GLU
1	A	79	ILE
1	A	86	THR
1	A	94	VAL
1	A	110	GLU

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Mol	Chain	Res	Type
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	133	ARG
1	A	136	GLU
1	A	141	SER
1	A	144	SER
1	A	145	PHE
1	A	155	SER
1	A	159	ARG
1	A	165	LEU
1	A	167	ASP
1	A	170	MET
1	A	175	GLN
1	A	177	LEU
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	219	ILE
1	A	242	MET
1	A	245	LYS
1	A	251	GLU
1	A	252	ARG
1	A	255	LYS
1	A	274	ARG
1	A	288	ARG
1	A	289	LEU
1	A	293	SER
1	A	297	PHE

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Mol	Chain	Res	Type
1	A	298	ILE
1	A	305	ASP
1	A	310	LEU

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

Mol	Chain	Res	Type
1	A	124	ASN
1	A	172	GLN
1	A	175	GLN
1	A	244	ASN
1	A	285	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 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 [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%)	-0.73	1 (0%) 94 84	2, 17, 55, 109	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	GLY	2.3

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 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.