



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 12, 2017 – 07:26 AM EST

PDB ID : 4NSW
Title : Crystal structure of the BAR-PH domain of ACAP1
Authors : Pang, X.; Zhang, K.; Ma, J.; Zhou, Q.; Sun, F.
Deposited on : unknown
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

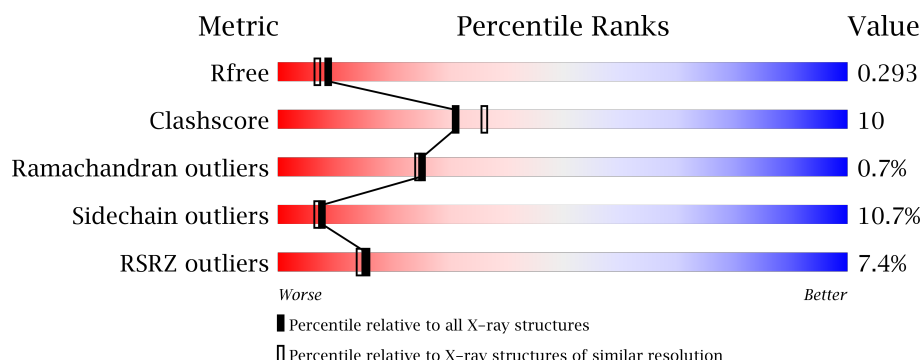
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	382	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• • •</div> </div> </div>
1	B	382	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>22%</div> <div>• 5%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5985 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 Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	0	0
			2940	1841	538	548	13			
1	B	362	Total	C	N	O	S	0	0	0
			2899	1813	532	541	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q15027
A	-3	PRO	-	EXPRESSION TAG	UNP Q15027
A	-2	LEU	-	EXPRESSION TAG	UNP Q15027
A	-1	GLY	-	EXPRESSION TAG	UNP Q15027
A	0	SER	-	EXPRESSION TAG	UNP Q15027
B	-4	GLY	-	EXPRESSION TAG	UNP Q15027
B	-3	PRO	-	EXPRESSION TAG	UNP Q15027
B	-2	LEU	-	EXPRESSION TAG	UNP Q15027
B	-1	GLY	-	EXPRESSION TAG	UNP Q15027
B	0	SER	-	EXPRESSION TAG	UNP Q15027

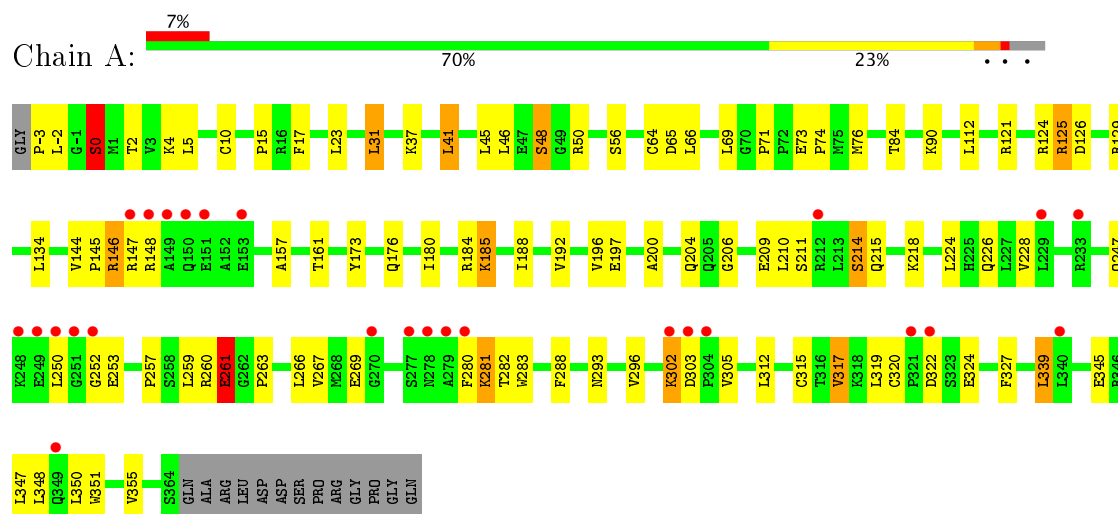
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	79	Total	O	0	0
			79	79		
2	B	67	Total	O	0	0
			67	67		

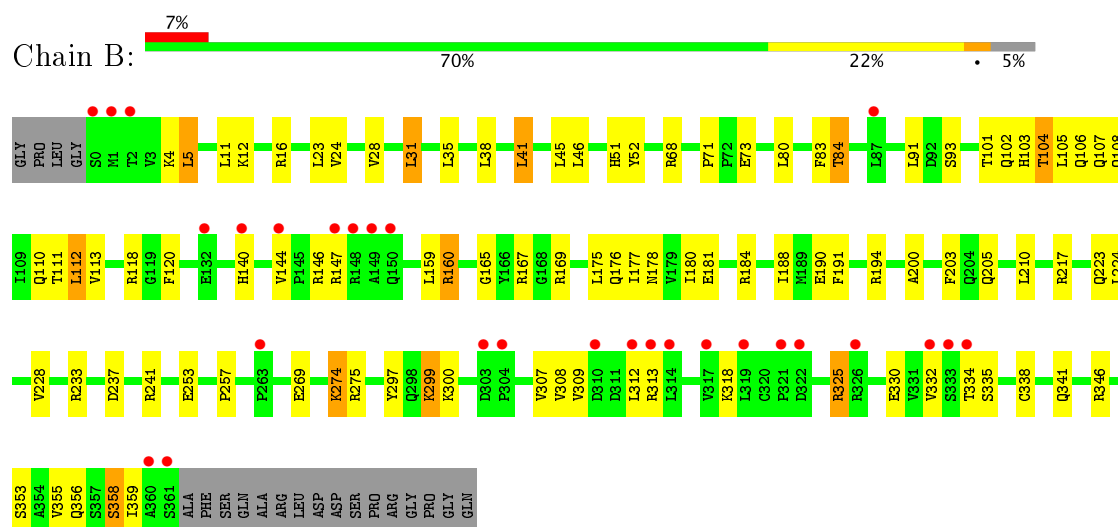
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1



- Molecule 1: Arf-GAP with coiled-coil, ANK repeat and PH domain-containing protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.46 Å 59.72 Å 168.95 Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	29.85 – 2.20 29.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.85-2.20) 95.3 (29.86-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.211 , 0.266 0.231 , 0.293	Depositor DCC
R_{free} test set	2059 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.570	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5985	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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	0.64	0/2989	0.75	5/4022 (0.1%)
1	B	0.66	0/2946	0.73	1/3964 (0.0%)
All	All	0.65	0/5935	0.74	6/7986 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	41	LEU	CB-CG-CD1	5.74	120.76	111.00
1	B	41	LEU	CA-CB-CG	5.56	128.10	115.30
1	A	31	LEU	CA-CB-CG	5.44	127.80	115.30
1	A	121	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	-2	LEU	CA-CB-CG	5.03	126.87	115.30

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	2940	0	2962	73	0
1	B	2899	0	2922	71	0
2	A	79	0	0	5	0
2	B	67	0	0	10	0
All	All	5985	0	5884	121	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 10.

All (121) 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:160:ARG:HH21	1:B:160:ARG:HG2	1.24	1.03
1:A:148:ARG:HG3	2:A:458:HOH:O	1.63	0.96
1:A:125:ARG:HD3	1:A:129:ARG:NH2	1.88	0.89
1:A:0:SER:HB2	1:B:71:PRO:HG3	1.55	0.86
1:B:159:LEU:HG	2:B:430:HOH:O	1.81	0.81
1:B:35:LEU:HD11	1:B:112:LEU:HD13	1.64	0.78
1:B:104:THR:HG23	1:B:194:ARG:HD3	1.66	0.77
1:B:160:ARG:CG	1:B:160:ARG:HH21	2.00	0.75
1:A:280:PHE:O	1:A:281:LYS:HB2	1.87	0.74
1:B:165:GLY:O	1:B:169:ARG:HG2	1.89	0.73
1:A:260:ARG:O	1:A:267:VAL:HG12	1.89	0.72
1:A:45:LEU:HD23	1:A:45:LEU:C	2.09	0.72
1:A:259:LEU:HB3	1:A:266:LEU:HD21	1.72	0.70
1:A:197:GLU:OE2	1:B:217:ARG:HD2	1.90	0.70
1:A:66:LEU:HD11	1:B:188:ILE:CD1	2.24	0.67
1:A:48:SER:OG	1:B:51:HIS:HD2	1.76	0.67
1:B:237:ASP:O	1:B:241:ARG:HG2	1.94	0.66
1:A:296:VAL:HB	1:A:305:VAL:HG13	1.77	0.66
1:A:66:LEU:HD11	1:B:188:ILE:HD11	1.78	0.66
1:A:327:PHE:HE2	1:A:345:GLU:HG2	1.62	0.65
1:A:71:PRO:HD2	1:B:184:ARG:NH1	2.12	0.64
1:A:48:SER:OG	1:B:51:HIS:CD2	2.51	0.64
1:A:211:SER:O	1:A:214:SER:HB3	1.99	0.63
1:A:66:LEU:C	1:A:66:LEU:HD13	2.19	0.63
1:A:327:PHE:CE2	1:A:345:GLU:HG2	2.35	0.62
1:B:312:LEU:HD23	1:B:358:SER:HB2	1.81	0.62
1:A:184:ARG:HD3	2:B:439:HOH:O	1.99	0.60
1:B:160:ARG:HG2	1:B:160:ARG:NH2	2.02	0.60
1:B:107:GLN:HG2	1:B:108:GLN:HE21	1.67	0.59
1:B:299:LYS:HG3	2:B:450:HOH:O	2.03	0.59
1:A:0:SER:CB	1:B:71:PRO:HG3	2.31	0.59
1:B:104:THR:HG22	1:B:108:GLN:HG2	1.84	0.58
1:B:105:LEU:HD22	1:B:191:PHE:HE1	1.68	0.58
1:A:224:LEU:O	1:A:228:VAL:HG23	2.04	0.58
1:B:355:VAL:O	1:B:359:ILE:HG13	2.03	0.57
1:A:185:LYS:NZ	2:A:453:HOH:O	2.37	0.57
1:B:140:HIS:O	1:B:144:VAL:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:NZ	1:A:209:GLU:HG2	2.19	0.57
1:A:351:TRP:O	1:A:355:VAL:HG23	2.05	0.56
1:A:252:GLY:HA3	1:B:160:ARG:HG3	1.87	0.56
1:A:317:VAL:HG21	1:A:355:VAL:CG1	2.35	0.56
1:A:250:LEU:HD12	1:A:252:GLY:HA2	1.86	0.56
1:B:102:GLN:O	1:B:106:GLN:HG3	2.05	0.56
1:A:250:LEU:HD13	1:B:167:ARG:HE	1.71	0.56
1:B:275:ARG:HD2	2:B:412:HOH:O	2.06	0.55
1:A:46:LEU:O	1:A:50:ARG:HG2	2.06	0.55
1:B:68:ARG:HD3	2:B:456:HOH:O	2.07	0.55
1:B:107:GLN:HG2	1:B:108:GLN:NE2	2.22	0.55
1:A:250:LEU:HD13	1:B:167:ARG:NE	2.21	0.55
1:A:64:CYS:SG	1:A:84:THR:HG21	2.47	0.54
1:A:253:GLU:O	1:B:167:ARG:NH2	2.40	0.54
1:B:309:VAL:HG11	1:B:312:LEU:HD12	1.88	0.54
1:A:125:ARG:HD2	1:A:126:ASP:OD1	2.07	0.53
1:A:125:ARG:HD3	1:A:129:ARG:HH22	1.70	0.53
1:B:176:GLN:NE2	2:B:453:HOH:O	2.42	0.53
1:B:224:LEU:O	1:B:228:VAL:HG23	2.09	0.53
1:A:125:ARG:CD	1:A:126:ASP:OD1	2.58	0.52
1:A:45:LEU:O	1:A:45:LEU:HD23	2.08	0.52
1:A:66:LEU:CD1	1:B:188:ILE:CD1	2.87	0.52
1:B:101:THR:O	1:B:105:LEU:HD23	2.10	0.52
1:B:118:ARG:NH1	2:B:449:HOH:O	2.24	0.52
1:A:257:PRO:HG2	1:A:350:LEU:HD23	1.91	0.52
1:A:192:VAL:HG12	1:B:83:PHE:HD1	1.75	0.51
1:B:103:HIS:HA	1:B:106:GLN:HE21	1.75	0.51
1:A:145:PRO:HB2	1:A:148:ARG:HD2	1.93	0.50
1:A:176:GLN:NE2	2:A:436:HOH:O	2.39	0.50
1:A:261:GLU:HB3	1:A:263:PRO:HD3	1.94	0.50
1:A:45:LEU:C	1:A:45:LEU:CD2	2.80	0.49
1:B:71:PRO:O	1:B:73:GLU:HG3	2.12	0.49
1:A:296:VAL:HB	1:A:305:VAL:CG1	2.44	0.48
1:A:69:LEU:HD11	1:B:31:LEU:N	2.29	0.48
1:A:125:ARG:HD3	1:A:129:ARG:HH21	1.74	0.48
1:B:312:LEU:CD2	1:B:358:SER:HB2	2.44	0.48
1:B:325:ARG:HH21	1:B:341:GLN:HE22	1.61	0.48
1:A:66:LEU:CD2	1:B:35:LEU:HD23	2.45	0.47
1:B:5:LEU:HD23	1:B:177:ILE:HG21	1.95	0.47
1:B:93:SER:OG	1:B:205:GLN:NE2	2.47	0.47
1:A:69:LEU:CD1	1:B:31:LEU:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ALA:O	1:A:161:THR:HG23	2.16	0.46
1:A:10:CYS:HB2	1:A:17:PHE:CE1	2.50	0.46
1:B:257:PRO:HB3	1:B:269:GLU:O	2.14	0.46
1:B:106:GLN:O	1:B:111:THR:HG23	2.15	0.46
1:B:274:LYS:HE3	1:B:297:TYR:CE2	2.51	0.46
1:A:260:ARG:HD3	1:A:269:GLU:OE1	2.15	0.45
1:A:206:GLY:HA3	1:B:203:PHE:CD1	2.51	0.45
1:A:15:PRO:HD2	2:A:429:HOH:O	2.16	0.45
1:B:178:ASN:HB2	2:B:421:HOH:O	2.16	0.45
1:B:80:LEU:O	1:B:84:THR:HG22	2.16	0.45
1:A:144:VAL:HA	1:A:145:PRO:HD3	1.72	0.45
1:A:146:ARG:HG3	1:A:147:ARG:HE	1.81	0.45
1:B:325:ARG:HE	1:B:341:GLN:NE2	2.15	0.45
1:A:196:VAL:HG21	1:B:83:PHE:CG	2.52	0.44
1:A:283:TRP:HH2	1:A:339:LEU:HD22	1.82	0.44
1:A:90:LYS:HZ2	1:A:209:GLU:HG2	1.81	0.44
1:A:317:VAL:HG21	1:A:355:VAL:HG12	1.99	0.44
1:B:11:LEU:HD22	1:B:167:ARG:HD3	1.98	0.43
1:B:346:ARG:HG2	1:B:346:ARG:HH11	1.83	0.43
1:B:35:LEU:HD12	1:B:113:VAL:CG1	2.48	0.43
1:B:110:GLN:HG3	2:B:420:HOH:O	2.19	0.43
1:B:353:SER:HA	1:B:356:GLN:HB2	2.01	0.42
1:A:48:SER:HB3	1:B:52:TYR:HA	2.01	0.42
1:A:261:GLU:C	1:A:263:PRO:HD3	2.40	0.42
1:A:293:ASN:HA	1:A:312:LEU:HD12	2.02	0.42
1:B:104:THR:HG22	1:B:108:GLN:CG	2.50	0.42
1:A:320:CYS:C	1:A:322:ASP:H	2.23	0.42
1:A:257:PRO:HD3	1:A:347:LEU:HD22	2.02	0.42
1:A:269:GLU:HA	1:A:288:PHE:O	2.19	0.42
1:A:124:ARG:HD3	2:A:435:HOH:O	2.20	0.41
1:B:24:VAL:HG11	1:B:177:ILE:HG12	2.02	0.41
1:A:73:GLU:HA	1:A:74:PRO:HD3	1.91	0.41
1:A:317:VAL:CG2	1:A:355:VAL:CG1	2.99	0.41
1:A:259:LEU:HD12	1:A:266:LEU:HD23	2.03	0.41
1:B:35:LEU:CD1	1:B:113:VAL:HG13	2.51	0.41
1:B:160:ARG:CG	1:B:160:ARG:NH2	2.69	0.41
1:B:180:ILE:HG23	2:B:453:HOH:O	2.20	0.41
1:A:302:LYS:HE3	1:A:303:ASP:HA	2.03	0.40
1:B:28:VAL:HG21	1:B:120:PHE:CZ	2.56	0.40
1:B:330:GLU:HG2	1:B:332:VAL:CG2	2.52	0.40
1:A:210:LEU:HD13	1:B:200:ALA:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ALA:HA	1:B:210:LEU:HD13	2.02	0.40
1:A:56:SER:HA	1:B:45:LEU:HD12	2.04	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	366/382 (96%)	347 (95%)	14 (4%)	5 (1%)	13	10
1	B	360/382 (94%)	352 (98%)	8 (2%)	0	100	100
All	All	726/764 (95%)	699 (96%)	22 (3%)	5 (1%)	25	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	281	LYS
1	A	146	ARG
1	A	261	GLU
1	A	247	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/325 (97%)	282 (90%)	33 (10%)	8	7
1	B	311/325 (96%)	277 (89%)	34 (11%)	7	6
All	All	626/650 (96%)	559 (89%)	67 (11%)	8	7

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-3	PRO
1	A	0	SER
1	A	2	THR
1	A	4	LYS
1	A	5	LEU
1	A	23	LEU
1	A	31	LEU
1	A	37	LYS
1	A	41	LEU
1	A	48	SER
1	A	65	ASP
1	A	76	MET
1	A	112	LEU
1	A	125	ARG
1	A	134	LEU
1	A	173	TYR
1	A	180	ILE
1	A	185	LYS
1	A	188	ILE
1	A	204	GLN
1	A	214	SER
1	A	215	GLN
1	A	218	LYS
1	A	226	GLN
1	A	261	GLU
1	A	282	THR
1	A	302	LYS
1	A	315	CYS
1	A	317	VAL
1	A	319	LEU
1	A	324	GLU
1	A	339	LEU
1	A	348	LEU
1	B	4	LYS
1	B	5	LEU

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Mol	Chain	Res	Type
1	B	12	LYS
1	B	16	ARG
1	B	23	LEU
1	B	31	LEU
1	B	38	LEU
1	B	41	LEU
1	B	46	LEU
1	B	84	THR
1	B	91	LEU
1	B	104	THR
1	B	112	LEU
1	B	146	ARG
1	B	147	ARG
1	B	160	ARG
1	B	175	LEU
1	B	181	GLU
1	B	190	GLU
1	B	223	GLN
1	B	233	ARG
1	B	253	GLU
1	B	274	LYS
1	B	299	LYS
1	B	300	LYS
1	B	307	VAL
1	B	308	VAL
1	B	313	ARG
1	B	318	LYS
1	B	325	ARG
1	B	334	THR
1	B	335	SER
1	B	338	CYS
1	B	358	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	226	GLN
1	A	271	HIS
1	A	341	GLN
1	B	51	HIS
1	B	88	ASN

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Mol	Chain	Res	Type
1	B	89	HIS
1	B	106	GLN
1	B	108	GLN
1	B	176	GLN
1	B	205	GLN
1	B	294	GLN
1	B	341	GLN

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 ⓘ

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	368/382 (96%)	0.44	26 (7%) 17 16	28, 56, 92, 124	0
1	B	362/382 (94%)	0.50	28 (7%) 14 13	28, 52, 102, 131	0
All	All	730/764 (95%)	0.47	54 (7%) 15 14	28, 53, 99, 131	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ARG	7.4
1	B	148	ARG	7.0
1	A	279	ALA	6.7
1	B	314	LEU	5.3
1	B	0	SER	5.0
1	B	263	PRO	4.9
1	A	149	ALA	4.6
1	A	280	PHE	4.5
1	B	1	MET	4.4
1	B	313	ARG	4.2
1	B	303	ASP	4.0
1	A	322	ASP	3.9
1	A	321	PRO	3.9
1	A	147	ARG	3.7
1	A	250	LEU	3.6
1	B	322	ASP	3.5
1	B	312	LEU	3.4
1	A	153	GLU	3.3
1	B	321	PRO	3.3
1	B	150	GLN	3.2
1	A	304	PRO	3.2
1	B	304	PRO	3.2
1	A	251	GLY	3.1
1	B	317	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	334	THR	3.0
1	A	150	GLN	2.9
1	B	132	GLU	2.8
1	B	144	VAL	2.7
1	A	248	LYS	2.7
1	B	140	HIS	2.6
1	B	361	SER	2.6
1	B	2	THR	2.6
1	A	302	LYS	2.6
1	A	233	ARG	2.6
1	A	278	ASN	2.6
1	B	149	ALA	2.5
1	A	229	LEU	2.4
1	A	249	GLU	2.3
1	B	332	VAL	2.3
1	A	151	GLU	2.3
1	A	252	GLY	2.3
1	A	349	GLN	2.3
1	A	148	ARG	2.3
1	B	360	ALA	2.2
1	B	319	LEU	2.2
1	B	333	SER	2.2
1	A	212	ARG	2.2
1	A	277	SER	2.1
1	B	87	LEU	2.1
1	A	270	GLY	2.1
1	A	303	ASP	2.0
1	A	340	LEU	2.0
1	B	326	ARG	2.0
1	B	310	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.