



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:40 AM UTC

PDB ID : 6H3A / pdb_00006h3a
Title : Crystal structure of the KAP1 RBCC domain in complex with the SMAR-CAD1 CUE1 domain.
Authors : Newman, J.A.; Aitkenhead, H.; Lim, M.; Williams, H.L.; Svejstrup, J.Q.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2018-07-17
Resolution : 5.50 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

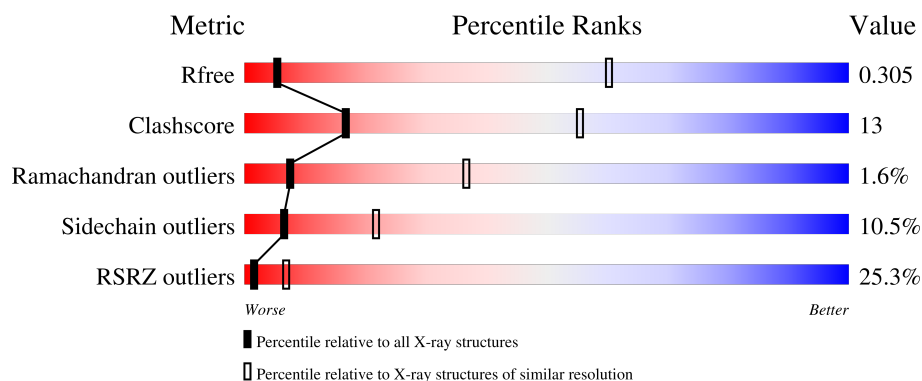
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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	B	253	6% 11% 8% . 77%
1	D	253	3% 9% 10% . 79%
2	A	382	18% 49% 19% . 30%
2	F	382	19% 49% 18% . 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5063 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 SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A containing DEAD/H box 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	53	Total	C	N	O	S	0	0	0
			389	243	61	83	2			
1	B	57	Total	C	N	O	S	0	0	0
			425	264	65	94	2			

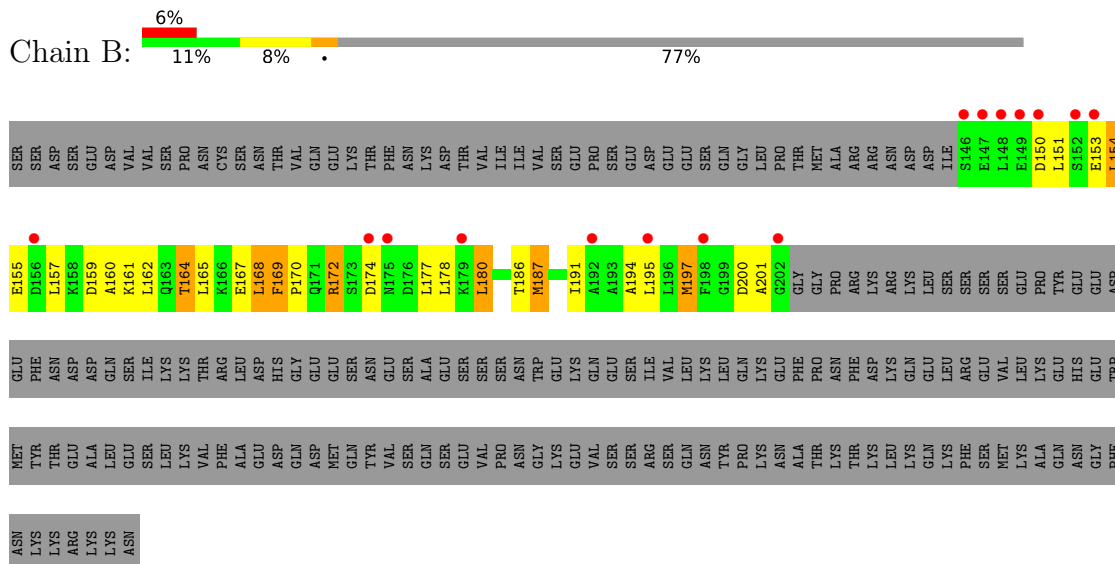
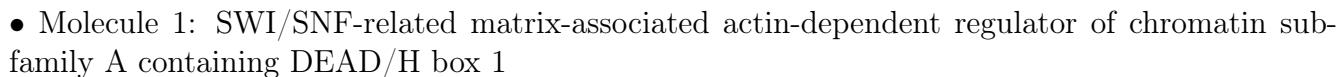
- Molecule 2 is a protein called Transcription intermediary factor 1-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	266	Total	C	N	O	S	0	0	0
			2115	1322	390	384	19			
2	F	268	Total	C	N	O	S	0	0	0
			2126	1329	392	386	19			

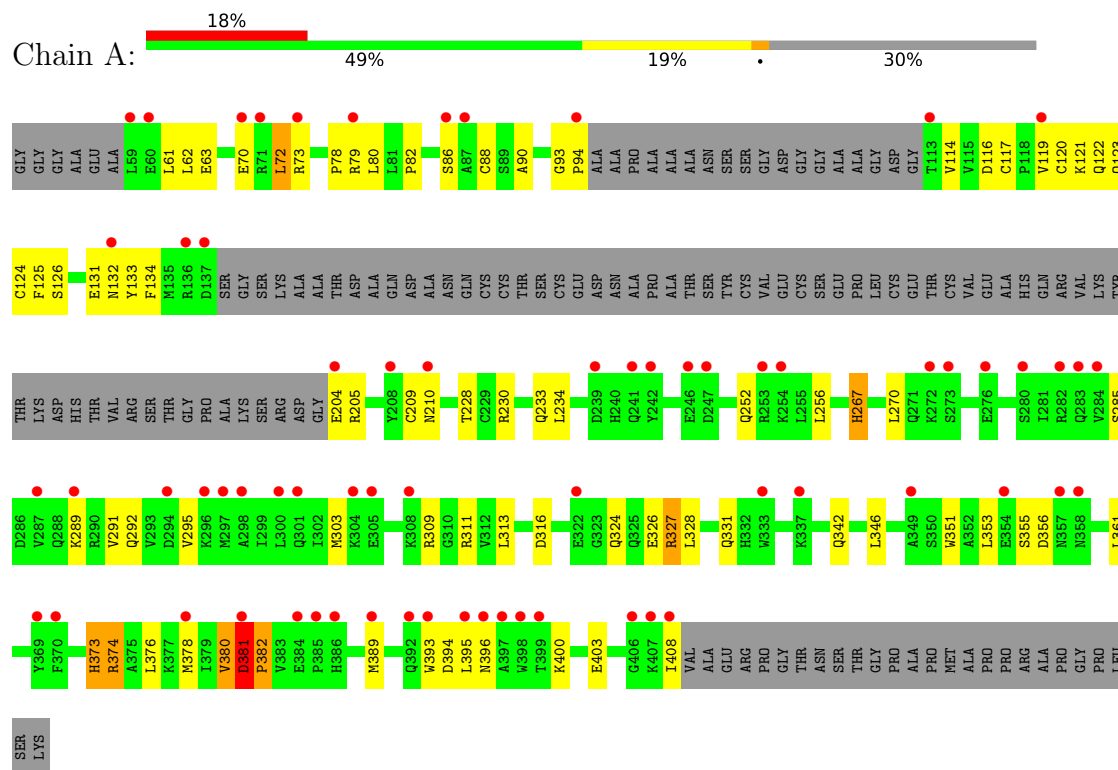
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Zn	0	0
			4	4		
3	F	4	Total	Zn	0	0
			4	4		

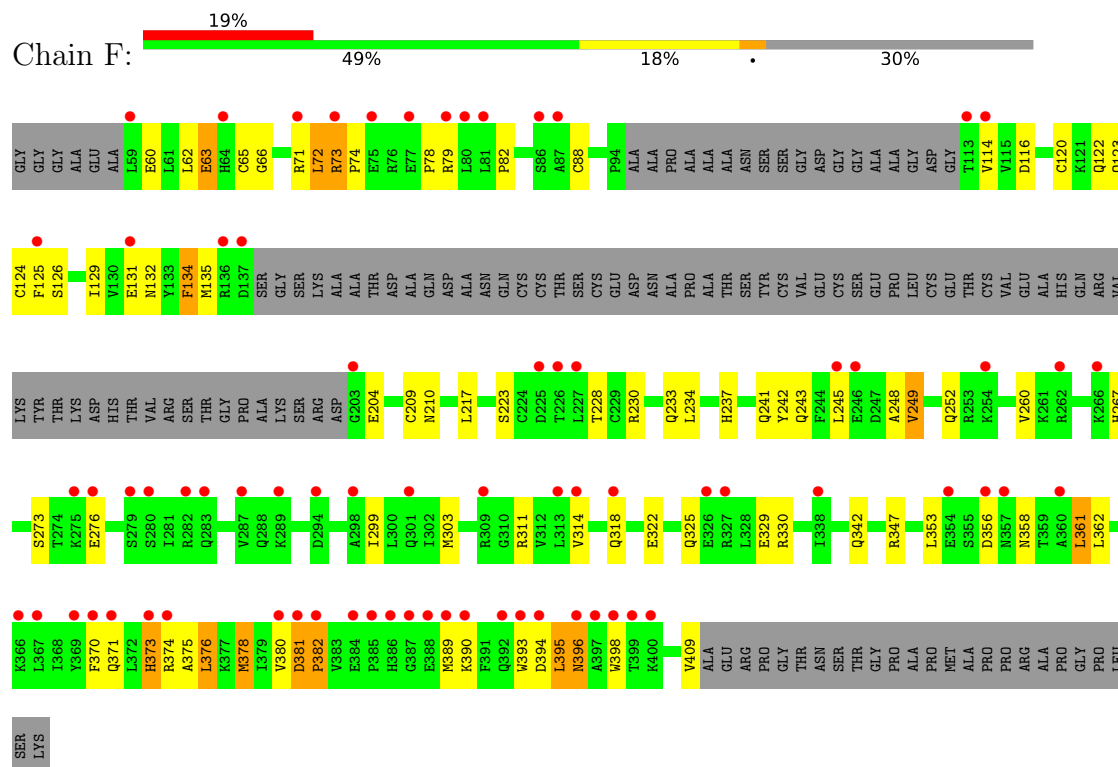
- Molecule 1: SWI/SNF-related matrix-associated actin-dependent regulator of chromatin subfamily A containing DEAD/H box 1



- Molecule 2: Transcription intermediary factor 1-beta



- Molecule 2: Transcription intermediary factor 1-beta



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	299.91Å 299.91Å 299.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.98 – 5.50 74.98 – 5.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (74.98-5.50) 99.9 (74.98-5.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 5.41Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.279 , 0.303 0.287 , 0.305	Depositor DCC
R_{free} test set	713 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	276.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 446.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.139 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5063	wwPDB-VP
Average B, all atoms (Å ²)	321.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	B	0.23	0/427	0.39	0/576
1	D	0.21	0/391	0.45	0/527
2	A	0.27	0/2151	0.50	0/2904
2	F	0.27	0/2162	0.50	0/2919
All	All	0.26	0/5131	0.49	0/6926

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	B	425	0	410	15	0
1	D	389	0	381	19	0
2	A	2115	0	2077	52	0
2	F	2126	0	2089	56	0
3	A	4	0	0	0	0
3	F	4	0	0	0	0
All	All	5063	0	4957	128	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 13.

All (128) 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)
2:F:374:ARG:O	2:F:378:MET:HB3	1.64	0.95
2:F:79:ARG:HA	2:F:131:GLU:HA	1.60	0.84
2:F:82:PRO:HG2	2:F:124:CYS:HB2	1.63	0.79
2:A:291:VAL:HG13	2:F:395:LEU:HD11	1.69	0.75
2:F:370:PHE:O	2:F:374:ARG:HB2	1.87	0.73
2:A:267:HIS:HA	2:A:270:LEU:HD12	1.70	0.73
2:A:82:PRO:HG2	2:A:124:CYS:HB2	1.74	0.70
1:D:169:PHE:HB2	1:D:195:LEU:HD11	1.74	0.68
1:B:177:LEU:HA	1:B:180:LEU:HD23	1.76	0.68
1:D:163:GLN:HB3	2:F:376:LEU:HD13	1.76	0.68
2:A:78:PRO:HA	2:A:88:CYS:HA	1.74	0.67
2:F:233:GLN:HA	2:F:237:HIS:HB2	1.77	0.67
2:F:228:THR:OG1	2:F:233:GLN:NE2	2.29	0.64
2:A:116:ASP:HA	2:A:122:GLN:HA	1.79	0.64
2:A:342:GLN:HE21	2:A:380:VAL:HG11	1.63	0.63
2:A:380:VAL:C	2:A:382:PRO:HD3	2.24	0.62
2:F:78:PRO:HA	2:F:88:CYS:HA	1.81	0.62
2:F:116:ASP:HA	2:F:122:GLN:HA	1.82	0.62
1:B:186:THR:HA	1:B:191:ILE:HD11	1.80	0.61
2:F:273:SER:HA	2:F:276:GLU:HB2	1.83	0.61
2:A:205:ARG:HB3	2:F:358:ASN:HB3	1.83	0.60
1:D:165:LEU:HD22	1:D:195:LEU:HD13	1.82	0.60
2:A:79:ARG:HA	2:A:131:GLU:HA	1.82	0.60
2:A:285:SER:HA	2:F:325:GLN:HE22	1.66	0.60
2:A:79:ARG:HA	2:A:132:ASN:H	1.67	0.60
2:F:65:CYS:SG	2:F:66:GLY:N	2.67	0.59
2:F:230:ARG:O	2:F:234:LEU:HG	2.04	0.57
1:D:169:PHE:CE1	1:D:200:ASP:HB3	2.40	0.57
1:D:194:ALA:HA	1:D:197:MET:HG3	1.84	0.57
1:B:200:ASP:OD1	1:B:201:ALA:N	2.24	0.57
2:F:375:ALA:HA	2:F:378:MET:SD	2.45	0.56
2:A:88:CYS:C	2:A:90:ALA:H	2.14	0.56
1:D:170:PRO:HB2	2:A:121:LYS:CB	2.36	0.56
2:A:327:ARG:HH11	2:A:327:ARG:HB2	1.71	0.56
2:F:361:LEU:H	2:F:361:LEU:HD23	1.69	0.56
2:A:61:LEU:HD11	2:F:347:ARG:NH1	2.22	0.55
2:A:204:GLU:N	2:A:204:GLU:OE1	2.41	0.53
2:F:342:GLN:HE21	2:F:380:VAL:HG11	1.72	0.53
1:D:196:LEU:HD22	1:D:201:ALA:HA	1.91	0.53
1:B:194:ALA:HA	1:B:197:MET:HE3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:374:ARG:O	2:F:378:MET:CB	2.48	0.52
1:D:160:ALA:O	1:D:164:THR:HG23	2.09	0.52
2:A:114:VAL:HG12	2:A:125:PHE:HA	1.91	0.52
2:A:63:GLU:O	2:A:72:LEU:HG	2.10	0.52
2:F:126:SER:HA	2:F:129:ILE:HD12	1.92	0.51
1:D:186:THR:HA	1:D:191:ILE:HD11	1.92	0.51
1:D:169:PHE:HD2	1:D:195:LEU:HD21	1.74	0.51
2:F:74:PRO:HB3	2:F:135:MET:HG2	1.93	0.51
2:F:396:ASN:N	2:F:396:ASN:OD1	2.43	0.51
2:A:88:CYS:SG	2:A:90:ALA:HB3	2.51	0.50
2:F:78:PRO:O	2:F:132:ASN:N	2.45	0.50
2:F:373:HIS:HA	2:F:376:LEU:HB2	1.91	0.50
1:B:169:PHE:HB2	1:B:195:LEU:HD11	1.93	0.50
1:D:162:LEU:HD22	1:D:178:LEU:HD21	1.94	0.49
2:A:327:ARG:HB2	2:A:327:ARG:NH1	2.28	0.49
2:F:135:MET:HB2	2:F:204:GLU:HG3	1.95	0.49
1:B:153:GLU:O	1:B:157:LEU:HG	2.13	0.49
2:F:318:GLN:O	2:F:322:GLU:HG2	2.12	0.49
1:D:153:GLU:O	1:D:157:LEU:HG	2.13	0.48
2:A:88:CYS:C	2:A:90:ALA:N	2.70	0.48
2:F:356:ASP:OD1	2:F:356:ASP:N	2.45	0.48
1:D:184:THR:O	1:D:185:SER:OG	2.30	0.48
2:A:295:VAL:HG11	2:F:314:VAL:HG22	1.95	0.48
2:A:373:HIS:HA	2:A:376:LEU:HB2	1.96	0.48
2:F:209:CYS:SG	2:F:210:ASN:N	2.87	0.48
1:B:161:LYS:HA	1:B:164:THR:HG23	1.96	0.47
2:A:78:PRO:O	2:A:132:ASN:N	2.47	0.47
2:F:381:ASP:N	2:F:382:PRO:HD3	2.29	0.47
2:A:351:TRP:NE1	2:F:62:LEU:HD12	2.29	0.47
2:A:93:GLY:H	2:A:94:PRO:HD2	1.79	0.47
2:A:351:TRP:HE1	2:F:62:LEU:HD12	1.79	0.47
2:F:204:GLU:N	2:F:204:GLU:OE1	2.47	0.47
2:F:373:HIS:CD2	2:F:376:LEU:HG	2.50	0.47
2:A:396:ASN:HB2	2:F:409:VAL:HG22	1.97	0.47
2:F:380:VAL:C	2:F:382:PRO:HD3	2.40	0.46
2:A:125:PHE:HD1	2:A:126:SER:H	1.62	0.46
1:B:162:LEU:HD22	1:B:178:LEU:HD21	1.97	0.46
2:A:381:ASP:N	2:A:382:PRO:HD3	2.31	0.46
1:D:154:LEU:HD22	1:D:154:LEU:H	1.80	0.46
1:B:165:LEU:HD22	1:B:195:LEU:HD13	1.98	0.46
2:A:228:THR:OG1	2:A:233:GLN:NE2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:LYS:O	1:D:170:PRO:HB3	2.16	0.45
2:A:209:CYS:SG	2:A:210:ASN:N	2.89	0.45
1:B:150:ASP:O	1:B:154:LEU:HD22	2.17	0.45
1:D:177:LEU:HA	1:D:180:LEU:HD23	1.99	0.45
2:F:63:GLU:H	2:F:63:GLU:HG2	1.57	0.45
2:F:361:LEU:HG	2:F:362:LEU:H	1.81	0.45
2:A:303:MET:HA	2:A:303:MET:HE2	1.99	0.44
2:A:309:ARG:O	2:A:313:LEU:HD13	2.17	0.44
2:A:289:LYS:O	2:A:292:GLN:HB3	2.18	0.44
2:A:353:LEU:HD22	2:F:260:VAL:HG21	2.00	0.44
2:A:408:ILE:HB	2:F:398:TRP:HH2	1.83	0.43
2:F:116:ASP:HB3	2:F:122:GLN:HB3	2.00	0.43
2:F:125:PHE:HD1	2:F:126:SER:H	1.66	0.43
2:A:400:LYS:O	2:A:403:GLU:HG3	2.18	0.43
1:B:168:LEU:O	1:B:170:PRO:HD3	2.17	0.43
2:F:248:ALA:O	2:F:252:GLN:HB2	2.18	0.43
2:A:324:GLN:O	2:A:328:LEU:HG	2.18	0.43
2:A:252:GLN:O	2:A:256:LEU:HG	2.19	0.43
2:A:355:SER:O	2:A:355:SER:OG	2.35	0.43
2:F:303:MET:HA	2:F:303:MET:HE2	2.00	0.42
2:A:327:ARG:HG2	2:A:331:GLN:NE2	2.34	0.42
1:B:172:ARG:H	1:B:172:ARG:HG2	1.43	0.42
2:A:117:CYS:SG	2:A:119:VAL:N	2.81	0.42
1:D:177:LEU:O	1:D:181:ILE:HG23	2.18	0.42
2:A:230:ARG:O	2:A:234:LEU:HG	2.19	0.42
2:F:223:SER:OG	2:F:241:GLN:HB2	2.20	0.42
2:F:114:VAL:HG12	2:F:125:PHE:HA	2.01	0.42
2:F:299:ILE:O	2:F:303:MET:HG2	2.19	0.42
2:A:205:ARG:H	2:A:205:ARG:HG3	1.63	0.42
2:F:228:THR:HG21	2:F:237:HIS:NE2	2.35	0.42
2:A:133:TYR:O	2:F:362:LEU:HD22	2.19	0.41
2:F:233:GLN:HG3	2:F:242:TYR:CZ	2.55	0.41
1:D:178:LEU:O	1:D:181:ILE:HG12	2.20	0.41
1:B:160:ALA:O	1:B:164:THR:HG23	2.20	0.41
2:F:233:GLN:HG3	2:F:242:TYR:CE1	2.54	0.41
2:A:376:LEU:HD12	1:B:167:GLU:HG3	2.01	0.41
2:F:72:LEU:HD13	2:F:134:PHE:HB3	2.02	0.41
2:A:80:LEU:HD12	2:A:86:SER:OG	2.20	0.41
2:F:371:GLN:HA	2:F:374:ARG:HB2	2.02	0.41
2:A:120:CYS:HB3	2:A:121:LYS:H	1.70	0.41
1:B:187:MET:HE2	1:B:187:MET:HB2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:71:ARG:O	2:F:73:ARG:N	2.53	0.41
2:F:245:LEU:O	2:F:249:VAL:N	2.44	0.40
1:D:172:ARG:H	1:D:172:ARG:HG2	1.47	0.40
2:A:63:GLU:H	2:A:63:GLU:HG2	1.66	0.40
2:A:356:ASP:OD1	2:A:356:ASP:N	2.52	0.40
2:A:374:ARG:O	2:A:378:MET:CB	2.70	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	B	55/253 (22%)	49 (89%)	4 (7%)	2 (4%)	2	20
1	D	51/253 (20%)	47 (92%)	3 (6%)	1 (2%)	6	30
2	A	260/382 (68%)	234 (90%)	23 (9%)	3 (1%)	10	43
2	F	262/382 (69%)	239 (91%)	19 (7%)	4 (2%)	8	39
All	All	628/1270 (49%)	569 (91%)	49 (8%)	10 (2%)	7	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	72	LEU
1	D	168	LEU
2	A	72	LEU
2	A	382	PRO
1	B	168	LEU
2	F	381	ASP
2	A	381	ASP
1	B	197	MET
2	F	120	CYS

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Mol	Chain	Res	Type
2	F	382	PRO

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	B	46/232 (20%)	36 (78%)	10 (22%)	1	6
1	D	41/232 (18%)	36 (88%)	5 (12%)	5	17
2	A	231/325 (71%)	211 (91%)	20 (9%)	9	29
2	F	232/325 (71%)	209 (90%)	23 (10%)	7	24
All	All	550/1114 (49%)	492 (90%)	58 (10%)	6	22

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

Mol	Chain	Res	Type
1	D	155	GLU
1	D	172	ARG
1	D	174	ASP
1	D	180	LEU
1	D	195	LEU
2	A	62	LEU
2	A	70	GLU
2	A	73	ARG
2	A	123	GLN
2	A	134	PHE
2	A	267	HIS
2	A	311	ARG
2	A	316	ASP
2	A	326	GLU
2	A	327	ARG
2	A	346	LEU
2	A	361	LEU
2	A	373	HIS
2	A	374	ARG
2	A	380	VAL

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Mol	Chain	Res	Type
2	A	381	ASP
2	A	389	MET
2	A	393	TRP
2	A	394	ASP
2	A	395	LEU
1	B	151	LEU
1	B	154	LEU
1	B	155	GLU
1	B	159	ASP
1	B	164	THR
1	B	169	PHE
1	B	172	ARG
1	B	174	ASP
1	B	180	LEU
1	B	187	MET
2	F	60	GLU
2	F	63	GLU
2	F	73	ARG
2	F	123	GLN
2	F	134	PHE
2	F	217	LEU
2	F	243	GLN
2	F	249	VAL
2	F	267	HIS
2	F	311	ARG
2	F	329	GLU
2	F	330	ARG
2	F	353	LEU
2	F	361	LEU
2	F	373	HIS
2	F	376	LEU
2	F	378	MET
2	F	389	MET
2	F	390	LYS
2	F	393	TRP
2	F	394	ASP
2	F	395	LEU
2	F	396	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	212	HIS
2	A	233	GLN
2	A	235	ASN
2	A	267	HIS
2	A	331	GLN
2	A	341	HIS
2	A	373	HIS
1	B	171	GLN
2	F	212	HIS
2	F	214	HIS
2	F	233	GLN
2	F	241	GLN
2	F	271	GLN
2	F	292	GLN
2	F	324	GLN
2	F	325	GLN
2	F	341	HIS
2	F	373	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](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	57/253 (22%)	1.32	15 (26%) 1 6	256, 297, 427, 446	0
1	D	53/253 (20%)	1.02	8 (15%) 5 12	279, 316, 373, 384	0
2	A	266/382 (69%)	1.24	67 (25%) 1 7	230, 317, 374, 449	0
2	F	268/382 (70%)	1.23	73 (27%) 1 6	196, 318, 406, 436	0
All	All	644/1270 (50%)	1.23	163 (25%) 1 7	196, 316, 398, 449	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	202	GLY	11.3
2	A	392	GLN	10.2
2	F	381	ASP	9.8
2	A	137	ASP	8.3
2	F	137	ASP	8.2
1	D	152	SER	6.9
2	A	408	ILE	6.8
2	F	392	GLN	6.5
2	F	389	MET	6.4
2	A	386	HIS	6.4
2	F	397	ALA	6.4
2	A	393	TRP	6.0
2	A	389	MET	5.9
2	F	380	VAL	5.5
1	D	203	GLY	5.3
1	B	146	SER	5.2
2	A	301	GLN	5.1
2	A	304	LYS	5.1
2	A	79	ARG	4.9
2	A	397	ALA	4.8
2	F	113	THR	4.7

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Mol	Chain	Res	Type	RSRZ
2	A	384	GLU	4.6
1	B	148	LEU	4.3
2	F	71	ARG	4.3
2	F	370	PHE	4.2
1	B	175	ASN	4.1
2	A	407	LYS	4.1
2	F	59	LEU	4.1
2	F	388	GLU	4.1
1	B	195	LEU	4.1
2	F	387	GLY	4.1
2	A	333	TRP	4.0
2	A	305	GLU	4.0
2	F	369	TYR	4.0
2	F	283	GLN	4.0
2	A	298	ALA	4.0
2	A	113	THR	3.9
2	A	354	GLU	3.8
2	F	136	ARG	3.7
2	A	406	GLY	3.7
2	A	59	LEU	3.7
2	A	253	ARG	3.7
2	F	396	ASN	3.6
2	F	386	HIS	3.6
1	D	171	GLN	3.6
2	F	279	SER	3.6
2	A	87	ALA	3.6
1	B	147	GLU	3.6
2	A	289	LYS	3.6
1	D	153	GLU	3.5
2	A	358	ASN	3.5
2	F	393	TRP	3.5
2	A	381	ASP	3.5
2	A	308	LYS	3.5
2	F	313	LEU	3.5
2	F	390	LYS	3.5
1	D	151	LEU	3.4
2	F	382	PRO	3.4
2	A	246	GLU	3.3
2	A	273	SER	3.3
2	F	373	HIS	3.3
2	F	79	ARG	3.3
2	F	282	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	156	ASP	3.3
2	A	287	VAL	3.2
2	A	272	LYS	3.2
2	F	225	ASP	3.2
2	F	125	PHE	3.2
2	A	322	GLU	3.2
2	F	287	VAL	3.2
2	F	246	GLU	3.1
1	D	175	ASN	3.1
2	A	254	LYS	3.1
2	F	226	THR	3.1
2	A	294	ASP	3.0
2	F	73	ARG	3.0
2	F	75	GLU	3.0
2	A	280	SER	3.0
2	F	400	LYS	2.9
2	F	131	GLU	2.9
2	A	86	SER	2.9
2	A	284	VAL	2.9
2	F	384	GLU	2.9
2	A	370	PHE	2.9
2	F	245	LEU	2.9
2	A	241	GLN	2.9
2	F	81	LEU	2.9
2	F	227	LEU	2.9
2	A	136	ARG	2.8
2	F	398	TRP	2.8
2	F	87	ALA	2.8
2	F	298	ALA	2.7
2	A	399	THR	2.7
2	F	371	GLN	2.7
1	B	150	ASP	2.7
2	F	203	GLY	2.7
2	A	73	ARG	2.7
2	F	366	LYS	2.7
2	F	275	LYS	2.7
2	F	294	ASP	2.6
1	B	153	GLU	2.6
2	A	296	LYS	2.6
1	B	152	SER	2.6
1	B	192	ALA	2.5
2	A	378	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	F	326	GLU	2.5
2	A	337	LYS	2.5
2	A	395	LEU	2.5
2	F	354	GLU	2.5
2	A	385	PRO	2.5
2	A	276	GLU	2.4
2	F	301	GLN	2.4
2	F	86	SER	2.4
2	A	297	MET	2.4
2	F	266	LYS	2.4
1	D	165	LEU	2.4
2	F	399	THR	2.4
2	F	114	VAL	2.4
2	F	367	LEU	2.4
2	A	60	GLU	2.4
2	A	71	ARG	2.4
2	A	119	VAL	2.4
2	F	374	ARG	2.4
2	F	357	ASN	2.3
2	F	360	ALA	2.3
2	A	247	ASP	2.3
2	F	80	LEU	2.3
2	F	289	LYS	2.3
2	F	385	PRO	2.3
2	F	394	ASP	2.3
1	B	149	GLU	2.3
1	B	174	ASP	2.3
2	F	309	ARG	2.2
2	F	318	GLN	2.2
1	B	198	PHE	2.2
2	A	204	GLU	2.2
1	D	185	SER	2.2
2	A	398	TRP	2.2
2	F	314	VAL	2.2
2	F	262	ARG	2.2
2	F	77	GLU	2.2
2	A	210	ASN	2.1
2	F	276	GLU	2.1
2	A	94	PRO	2.1
2	F	338	ILE	2.1
2	A	70	GLU	2.1
2	A	369	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	356	ASP	2.1
2	A	357	ASN	2.1
2	F	64	HIS	2.1
2	F	254	LYS	2.1
2	F	280	SER	2.1
2	A	239	ASP	2.1
1	B	179	LYS	2.1
2	A	349	ALA	2.1
2	A	396	ASN	2.1
2	A	283	GLN	2.1
2	A	242	TYR	2.0
2	A	300	LEU	2.0
2	A	132	ASN	2.0
2	A	282	ARG	2.0
2	A	208	TYR	2.0
2	F	327	ARG	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1001	1/1	0.99	0.05	200,200,200,200	0
3	ZN	A	1004	1/1	0.99	0.04	346,346,346,346	0
3	ZN	F	501	1/1	0.99	0.07	279,279,279,279	0
3	ZN	F	503	1/1	0.99	0.05	327,327,327,327	0
3	ZN	F	504	1/1	0.99	0.09	256,256,256,256	0
3	ZN	F	502	1/1	1.00	0.02	262,262,262,262	0
3	ZN	A	1002	1/1	1.00	0.07	274,274,274,274	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	A	1003	1/1	1.00	0.03	225,225,225,225	0

6.5 Other polymers [i](#)

There are no such residues in this entry.