



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 10:53 PM UTC

PDB ID : 2BAP / pdb_00002bap
Title : Crystal structure of the N-terminal mDial Armadillo Repeat Region and Dimerisation Domain in complex with the mDial autoregulatory domain (DAD)
Authors : Lammers, M.; Rose, R.; Scrima, A.; Wittinghofer, A.
Deposited on : 2005-10-14
Resolution : 3.30 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

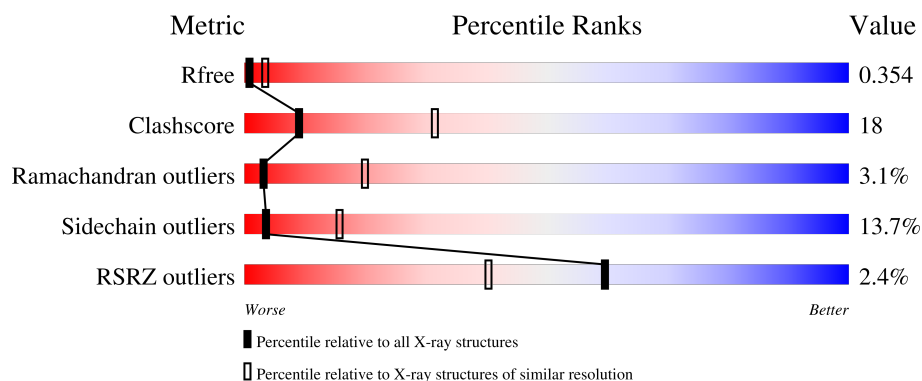
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	317	3% 50% 35% 9% 7%
1	B	317	% 56% 31% 5% 7%
2	C	56	18% 11% 71%
2	D	56	4% 18% 11% 71%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4960 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.

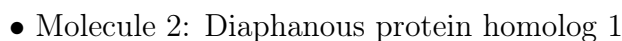
- Molecule 1 is a protein called Diaphanous protein homolog 1.

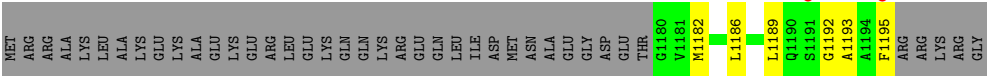
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	294	Total	C	N	O	S	0	0	0
			2363	1490	404	448	21			
1	A	295	Total	C	N	O	S	0	0	0
			2375	1499	405	450	21			

- Molecule 2 is a protein called Diaphanous protein homolog 1.

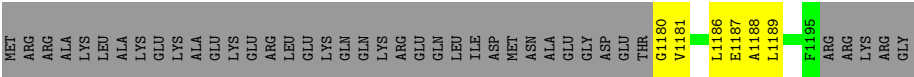
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	S	0	0	0
			111	70	17	23	1			
2	C	16	Total	C	N	O	S	0	0	0
			111	70	17	23	1			

- Molecule 1: Diaphanous protein homolog 1





● Molecule 2: Diaphanous protein homolog 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.45Å 138.45Å 210.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.98 – 3.30 19.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-3.30) 99.3 (19.98-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.21 (at 3.29Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.288 , 0.364 0.285 , 0.354	Depositor DCC
R_{free} test set	925 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4960	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.93% 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	0.69	1/2408 (0.0%)	1.00	6/3242 (0.2%)
1	B	0.50	0/2395	0.93	2/3224 (0.1%)
2	C	0.47	0/111	0.83	0/148
2	D	0.48	0/111	0.83	0/148
All	All	0.60	1/5025 (0.0%)	0.96	8/6762 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	HIS	C-O	20.06	1.63	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	HIS	CA-C-O	-8.75	105.92	120.80
1	B	382	GLY	N-CA-C	-7.36	103.97	112.50
1	A	351	VAL	N-CA-C	-6.46	106.44	112.83
1	A	314	THR	CA-C-N	-5.42	114.43	120.45
1	A	314	THR	C-N-CA	-5.42	114.43	120.45
1	A	201	ASP	N-CA-C	5.35	116.86	110.44
1	B	393	LYS	N-CA-C	5.16	116.59	111.07
1	A	202	SER	N-CA-C	-5.02	105.90	112.23

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	A	2375	0	2395	98	0
1	B	2363	0	2386	82	0
2	C	111	0	108	5	0
2	D	111	0	108	6	0
All	All	4960	0	4997	183	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 18.

All (183) 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:435:HIS:O	1:A:435:HIS:C	1.63	1.40
1:A:239:MET:CE	1:A:254:LEU:HD12	1.79	1.12
1:B:263:PRO:HB2	1:B:266:MET:HE3	1.24	1.10
1:A:421:TYR:HE1	1:A:425:ILE:HD11	1.12	1.06
1:A:239:MET:HE1	1:A:254:LEU:HD12	1.45	0.99
1:A:402:LEU:O	1:A:406:GLN:HG3	1.65	0.95
1:A:421:TYR:CE1	1:A:425:ILE:HD11	2.02	0.94
1:B:263:PRO:HB2	1:B:266:MET:CE	1.98	0.93
1:A:244:PRO:O	1:A:248:ILE:HG12	1.70	0.91
1:A:303:VAL:O	1:A:307:GLN:HB2	1.75	0.87
1:B:403:SER:HA	1:B:406:GLN:HE21	1.40	0.84
1:A:400:HIS:O	1:A:403:SER:OG	1.95	0.82
1:A:239:MET:HE3	1:A:254:LEU:HD12	1.62	0.81
1:B:216:MET:HE2	1:B:225:MET:HG2	1.67	0.76
1:B:417:ALA:HA	1:B:420:GLN:OE1	1.87	0.75
1:A:421:TYR:HE1	1:A:425:ILE:CD1	1.97	0.74
1:A:346:ASN:HB3	1:A:349:MET:HB3	1.68	0.74
1:B:263:PRO:O	1:B:266:MET:HG2	1.87	0.73
1:B:380:ASP:HB2	1:B:383:GLU:HG2	1.71	0.72
1:A:239:MET:HE3	1:A:254:LEU:CD1	2.20	0.71
1:A:378:MET:HG2	1:A:384:VAL:HG23	1.72	0.71
1:B:161:VAL:HG21	1:A:161:VAL:HG11	1.72	0.70
1:A:239:MET:CE	1:A:254:LEU:CD1	2.66	0.70
1:A:427:GLU:HA	1:A:430:SER:OG	1.92	0.69
1:A:182:LEU:HD22	1:A:208:ILE:HG23	1.77	0.65
1:B:213:LYS:HA	1:B:253:LEU:HD21	1.77	0.65
1:A:425:ILE:O	1:A:429:VAL:HG12	1.96	0.65
1:A:345:GLU:HA	1:A:350:LYS:HZ2	1.62	0.65
1:B:232:ILE:HD12	1:B:232:ILE:H	1.62	0.64
1:A:212:LEU:HB3	1:A:216:MET:HE2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ILE:HD13	1:A:301:LEU:HA	1.80	0.63
1:B:182:LEU:HD22	1:B:208:ILE:HG23	1.80	0.62
1:B:380:ASP:HB3	1:B:383:GLU:H	1.65	0.61
1:A:396:LYS:O	1:A:399:PRO:HD2	1.99	0.61
1:A:418:ARG:N	1:A:419:PRO:HD2	2.14	0.61
1:B:355:VAL:HG21	2:D:1195:PHE:CB	2.29	0.61
1:A:245:ASN:HA	1:A:248:ILE:HG13	1.82	0.61
1:B:263:PRO:CB	1:B:266:MET:HE3	2.15	0.61
1:B:420:GLN:O	1:B:424:LEU:HG	2.01	0.60
1:B:177:GLU:H	1:B:177:GLU:CD	2.09	0.60
1:A:429:VAL:O	1:A:433:VAL:HG23	2.00	0.60
1:B:212:LEU:HB3	1:B:216:MET:HE3	1.83	0.60
1:A:378:MET:HG2	1:A:384:VAL:CG2	2.32	0.60
2:C:1187:GLU:C	2:C:1189:LEU:H	2.10	0.59
1:A:249:ASP:O	1:A:253:LEU:HB2	2.01	0.59
1:A:148:ARG:O	1:A:152:LEU:HB2	2.02	0.59
1:B:380:ASP:O	1:B:381:PHE:HB2	2.02	0.59
1:B:359:GLN:HE21	1:B:359:GLN:HA	1.68	0.59
1:A:345:GLU:HA	1:A:350:LYS:NZ	2.17	0.59
1:B:378:MET:HA	1:B:383:GLU:HB3	1.86	0.58
1:B:266:MET:HE1	1:B:269:ARG:HH21	1.69	0.58
1:A:179:LEU:HG	1:A:215:PHE:CE2	2.40	0.57
1:B:257:LEU:HA	1:B:260:LEU:HD13	1.85	0.57
1:A:321:PHE:O	1:A:324:HIS:HB3	2.04	0.57
1:A:217:ASN:ND2	2:C:1180:GLY:HA2	2.20	0.56
1:A:177:GLU:H	1:A:177:GLU:CD	2.13	0.56
1:B:226:LEU:HD21	1:B:257:LEU:HD22	1.87	0.55
1:B:297:THR:OG1	1:B:302:LYS:HE3	2.06	0.55
1:B:144:ARG:HH22	1:B:177:GLU:HB3	1.72	0.55
1:A:142:GLU:O	1:A:147:LEU:HG	2.07	0.55
1:B:255:SER:HB3	1:B:308:LEU:HA	1.88	0.54
1:A:359:GLN:HE21	1:A:359:GLN:HA	1.74	0.53
1:B:233:LEU:O	1:B:237:ARG:HG2	2.07	0.53
1:A:421:TYR:C	1:A:421:TYR:CD1	2.86	0.53
1:A:372:ASP:HA	1:A:375:ARG:HG3	1.91	0.52
1:B:403:SER:HA	1:B:406:GLN:NE2	2.16	0.52
1:B:374:ILE:HG23	1:B:378:MET:HE3	1.91	0.52
1:A:166:ASN:HD22	1:A:167:PRO:HD2	1.76	0.51
1:B:418:ARG:N	1:B:419:PRO:HD2	2.26	0.50
1:A:435:HIS:O	1:A:435:HIS:CA	2.56	0.50
1:A:216:MET:O	1:A:218:ASN:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:HD23	1:A:434:LEU:HD23	1.93	0.50
1:A:420:GLN:O	1:A:423:LYS:HB3	2.12	0.50
1:A:407:HIS:HA	1:A:410:LEU:HD12	1.93	0.50
1:A:239:MET:HE1	1:A:308:LEU:HD11	1.94	0.49
1:A:239:MET:O	1:A:240:ASP:HB3	2.11	0.49
1:B:240:ASP:H	1:B:247:MET:HB2	1.77	0.49
1:B:421:TYR:CE1	1:B:425:ILE:HG13	2.48	0.49
1:A:403:SER:HA	1:A:406:GLN:HE21	1.78	0.49
1:B:415:TYR:CZ	1:B:417:ALA:HB3	2.48	0.49
1:B:339:GLN:O	1:B:342:ARG:HG3	2.13	0.48
1:A:405:LEU:HA	1:A:408:LEU:HD12	1.95	0.48
1:A:266:MET:SD	1:A:269:ARG:HD3	2.54	0.48
1:B:150:MET:SD	1:A:138:MET:HG3	2.53	0.48
1:B:289:LEU:HD21	1:B:308:LEU:HD23	1.96	0.48
1:A:275:THR:HG23	1:A:285:ARG:HD3	1.96	0.48
1:B:222:ILE:HG21	1:B:260:LEU:HD21	1.95	0.48
1:A:423:LYS:O	1:A:426:GLU:HB3	2.14	0.47
1:B:330:MET:HE3	1:B:334:LEU:HD23	1.96	0.47
1:A:429:VAL:HA	1:A:432:ILE:HD12	1.96	0.47
1:B:216:MET:C	1:B:218:ASN:H	2.23	0.47
1:B:271:LEU:HD22	1:B:312:LEU:HD22	1.96	0.47
1:A:185:ILE:O	1:A:189:LEU:HB2	2.15	0.47
1:B:334:LEU:O	1:B:338:LEU:HB2	2.15	0.47
1:A:257:LEU:O	1:A:260:LEU:HB2	2.15	0.47
1:A:427:GLU:C	1:A:430:SER:HG	2.23	0.47
1:A:243:VAL:O	1:A:243:VAL:HG12	2.15	0.47
1:A:236:VAL:HG11	1:A:274:MET:HA	1.97	0.46
1:A:177:GLU:O	1:A:180:ALA:HB3	2.14	0.46
1:A:201:ASP:OD2	1:A:204:ASN:ND2	2.48	0.46
1:A:421:TYR:C	1:A:421:TYR:HD1	2.23	0.46
1:B:346:ASN:ND2	1:B:348:ASP:H	2.13	0.46
1:A:248:ILE:CD1	1:A:301:LEU:HA	2.46	0.46
1:A:380:ASP:HB3	1:A:383:GLU:HG2	1.98	0.46
1:B:236:VAL:HG11	1:B:274:MET:HA	1.98	0.46
1:A:368:LYS:HD2	1:A:371:LEU:HD23	1.96	0.46
2:D:1182:MET:HE3	2:D:1186:LEU:HG	1.97	0.46
1:B:206:HIS:HD1	1:B:206:HIS:C	2.24	0.46
1:B:359:GLN:HE21	1:B:359:GLN:CA	2.30	0.45
1:A:216:MET:HB3	1:A:222:ILE:HG23	1.98	0.45
1:A:364:PHE:CD2	1:A:364:PHE:C	2.95	0.45
1:B:144:ARG:C	1:B:146:GLY:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:HB	1:A:301:LEU:HD23	1.98	0.45
1:B:373:ASP:C	1:B:375:ARG:H	2.23	0.45
1:A:395:SER:O	1:A:397:ALA:N	2.50	0.45
1:B:421:TYR:O	1:B:424:LEU:HB2	2.17	0.45
1:B:162:SER:O	1:B:166:ASN:ND2	2.44	0.45
1:A:274:MET:HE3	1:A:274:MET:HB2	1.74	0.45
1:B:378:MET:O	1:B:378:MET:HG2	2.17	0.45
1:B:204:ASN:H	1:B:204:ASN:HD22	1.63	0.45
1:A:193:LYS:HD3	1:A:193:LYS:N	2.32	0.45
1:A:392:VAL:HG11	1:A:401:PHE:CG	2.52	0.44
1:A:395:SER:C	1:A:397:ALA:H	2.24	0.44
1:A:232:ILE:H	1:A:232:ILE:HG13	1.56	0.44
1:B:189:LEU:HD13	1:B:205:GLN:HB3	1.98	0.44
1:A:428:CYS:O	1:A:432:ILE:HG13	2.18	0.44
2:C:1187:GLU:C	2:C:1189:LEU:N	2.76	0.44
2:C:1186:LEU:O	2:C:1189:LEU:HB3	2.18	0.44
1:A:218:ASN:HA	2:C:1181:VAL:HB	2.00	0.44
1:A:417:ALA:O	1:A:420:GLN:HB2	2.18	0.44
1:B:389:LEU:HA	1:B:393:LYS:HB2	2.00	0.43
1:B:405:LEU:HA	1:B:408:LEU:HD12	2.00	0.43
1:A:258:CYS:C	1:A:260:LEU:H	2.26	0.43
1:A:319:LEU:O	1:A:323:VAL:HG12	2.19	0.43
1:B:373:ASP:C	1:B:375:ARG:N	2.74	0.43
1:A:392:VAL:O	1:A:392:VAL:HG12	2.18	0.43
1:A:403:SER:O	1:A:404:ILE:C	2.62	0.43
1:B:148:ARG:HD3	1:B:148:ARG:HA	1.76	0.43
1:A:413:ASN:O	1:A:418:ARG:NH1	2.52	0.43
1:B:147:LEU:O	1:B:148:ARG:NH1	2.52	0.43
1:A:321:PHE:O	1:A:325:ILE:HG13	2.18	0.43
1:B:160:ARG:HG3	1:B:161:VAL:H	1.84	0.43
1:A:395:SER:C	1:A:397:ALA:N	2.75	0.42
1:B:248:ILE:HG22	1:B:252:LYS:HE2	2.01	0.42
1:A:243:VAL:O	1:A:244:PRO:C	2.62	0.42
1:A:222:ILE:HD12	1:A:223:LYS:N	2.33	0.42
1:B:286:PHE:CE1	1:B:328:GLU:HG2	2.55	0.42
1:B:279:GLU:O	1:B:280:MET:C	2.62	0.42
1:B:310:ASN:ND2	1:B:355:VAL:HG12	2.34	0.42
1:A:248:ILE:HG12	1:A:248:ILE:H	1.71	0.42
1:A:386:GLN:O	1:A:390:ASN:ND2	2.52	0.42
1:A:260:LEU:HA	1:A:261:PRO:HD3	1.74	0.42
1:A:404:ILE:HG22	1:A:408:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:VAL:HG21	2:D:1195:PHE:HB3	2.01	0.42
1:B:260:LEU:HA	1:B:261:PRO:HD3	1.67	0.42
1:B:421:TYR:CD1	1:B:421:TYR:C	2.98	0.42
1:A:243:VAL:HG11	1:A:246:MET:HE2	2.01	0.42
1:B:243:VAL:HG12	1:B:243:VAL:O	2.19	0.41
1:B:259:ILE:HD11	2:D:1189:LEU:HD21	2.02	0.41
1:B:341:LEU:O	1:B:353:LEU:HD11	2.20	0.41
1:A:254:LEU:HA	1:A:257:LEU:HD12	2.02	0.41
1:B:355:VAL:HG21	2:D:1195:PHE:HB2	2.02	0.41
1:B:346:ASN:HD22	1:B:348:ASP:H	1.67	0.41
1:A:217:ASN:O	1:A:218:ASN:HB3	2.20	0.41
1:A:278:ALA:HB1	1:A:283:VAL:O	2.20	0.41
1:B:321:PHE:C	1:B:321:PHE:CD2	2.98	0.41
1:A:233:LEU:O	1:A:237:ARG:HG3	2.21	0.41
1:B:166:ASN:HB3	1:B:167:PRO:HD2	2.03	0.41
2:D:1193:ALA:C	2:D:1195:PHE:H	2.29	0.41
1:B:147:LEU:HB3	1:B:148:ARG:H	1.80	0.41
1:B:216:MET:HE2	1:B:225:MET:CG	2.43	0.41
1:B:260:LEU:HB3	1:B:263:PRO:HD2	2.03	0.41
1:B:216:MET:CE	1:B:225:MET:HG2	2.44	0.41
1:B:290:LEU:HD13	1:B:290:LEU:HA	1.98	0.41
1:B:388:ILE:O	1:B:392:VAL:HB	2.21	0.41
1:A:222:ILE:HD12	1:A:223:LYS:H	1.85	0.41
1:A:248:ILE:O	1:A:252:LYS:HG2	2.21	0.41
1:B:303:VAL:O	1:B:307:GLN:HB2	2.20	0.40
1:B:216:MET:O	1:B:222:ILE:HG13	2.20	0.40
1:B:257:LEU:O	1:B:260:LEU:HB2	2.21	0.40
1:A:260:LEU:HD23	1:A:263:PRO:CG	2.52	0.40
1:A:418:ARG:N	1:A:419:PRO:CD	2.84	0.40
1:B:421:TYR:HE1	1:B:425:ILE:HG13	1.86	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	291/317 (92%)	237 (81%)	47 (16%)	7 (2%)	4	24
1	B	290/317 (92%)	248 (86%)	32 (11%)	10 (3%)	3	18
2	C	14/56 (25%)	11 (79%)	2 (14%)	1 (7%)	1	6
2	D	14/56 (25%)	10 (71%)	3 (21%)	1 (7%)	1	6
All	All	609/746 (82%)	506 (83%)	84 (14%)	19 (3%)	3	20

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	LEU
1	B	411	VAL
1	A	217	ASN
1	A	219	LYS
1	A	231	GLY
1	B	262	GLN
1	B	145	SER
1	B	282	GLU
2	D	1192	GLY
2	C	1188	ALA
1	B	217	ASN
1	B	231	GLY
1	A	411	VAL
1	A	175	GLY
1	A	259	ILE
1	B	146	GLY
1	B	244	PRO
1	B	374	ILE
1	A	240	ASP

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	267/287 (93%)	223 (84%)	44 (16%)	2	11
1	B	266/287 (93%)	234 (88%)	32 (12%)	5	20
2	C	11/45 (24%)	11 (100%)	0	100	100
2	D	11/45 (24%)	11 (100%)	0	100	100
All	All	555/664 (84%)	479 (86%)	76 (14%)	3	16

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	143	LEU
1	B	149	ASP
1	B	153	LEU
1	B	177	GLU
1	B	186	LEU
1	B	193	LYS
1	B	201	ASP
1	B	233	LEU
1	B	237	ARG
1	B	245	ASN
1	B	255	SER
1	B	271	LEU
1	B	277	ARG
1	B	281	ASP
1	B	283	VAL
1	B	290	LEU
1	B	297	THR
1	B	317	GLU
1	B	328	GLU
1	B	330	MET
1	B	342	ARG
1	B	354	CYS
1	B	355	VAL
1	B	359	GLN
1	B	374	ILE
1	B	377	GLU
1	B	378	MET
1	B	380	ASP
1	B	386	GLN
1	B	414	ASP
1	B	423	LYS
1	B	427	GLU
1	A	137	MET

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Mol	Chain	Res	Type
1	A	138	MET
1	A	143	LEU
1	A	152	LEU
1	A	153	LEU
1	A	161	VAL
1	A	173	THR
1	A	179	LEU
1	A	181	SER
1	A	189	LEU
1	A	193	LYS
1	A	201	ASP
1	A	205	GLN
1	A	222	ILE
1	A	224	THR
1	A	225	MET
1	A	232	ILE
1	A	248	ILE
1	A	249	ASP
1	A	262	GLN
1	A	275	THR
1	A	287	GLN
1	A	297	THR
1	A	308	LEU
1	A	319	LEU
1	A	323	VAL
1	A	325	ILE
1	A	327	SER
1	A	329	LEU
1	A	330	MET
1	A	354	CYS
1	A	359	GLN
1	A	371	LEU
1	A	374	ILE
1	A	376	MET
1	A	377	GLU
1	A	386	GLN
1	A	387	ILE
1	A	396	LYS
1	A	402	LEU
1	A	411	VAL
1	A	414	ASP
1	A	429	VAL

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Mol	Chain	Res	Type
1	A	433	VAL

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

Mol	Chain	Res	Type
1	B	172	GLN
1	B	190	HIS
1	B	324	HIS
1	B	346	ASN
1	B	359	GLN
1	B	406	GLN
1	A	164	ASN
1	A	166	ASN
1	A	190	HIS
1	A	346	ASN
1	A	359	GLN
1	A	390	ASN
1	A	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	295/317 (93%)	0.43	9 (3%) 51 35	29, 95, 108, 114	0
1	B	294/317 (92%)	0.23	4 (1%) 73 55	29, 93, 105, 112	0
2	C	16/56 (28%)	0.67	0 100 100	114, 116, 117, 118	0
2	D	16/56 (28%)	0.72	2 (12%) 8 6	112, 115, 116, 117	0
All	All	621/746 (83%)	0.35	15 (2%) 59 40	29, 95, 113, 118	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	SER	4.5
1	B	135	SER	3.9
1	B	331	ARG	3.8
1	A	353	LEU	3.0
1	B	424	LEU	2.9
1	A	242	ALA	2.8
2	D	1195	PHE	2.7
1	A	216	MET	2.4
1	A	150	MET	2.3
1	A	306	LEU	2.2
1	A	321	PHE	2.2
1	B	413	ASN	2.2
1	A	274	MET	2.2
1	A	249	ASP	2.1
2	D	1191	SER	2.1

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.