



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:14 AM UTC

PDB ID : 3ANR / pdb_00003anr
Title : human DYRK1A/harmine complex
Authors : Nonaka, Y.; Hosoya, T.; Hagiwara, M.; Ito, N.
Deposited on : 2010-09-06
Resolution : 2.60 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

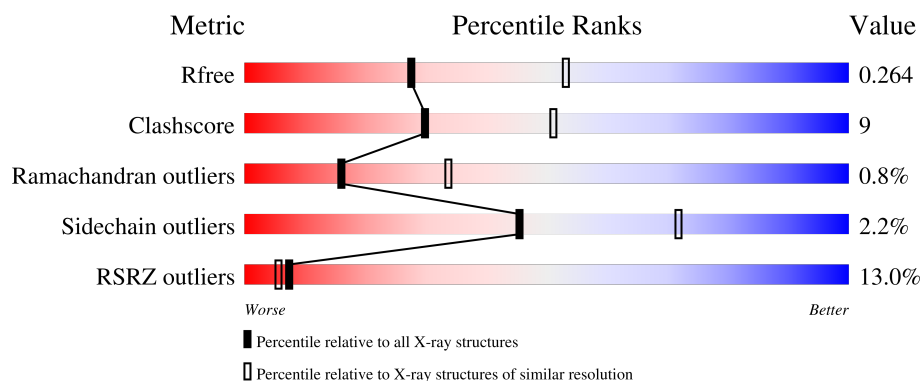
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	368	4% 74% 18% • 7%
1	B	368	12% 75% 16% • 7%
1	C	368	26% 72% 18% • 8%
1	D	368	7% 73% 19% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11266 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.

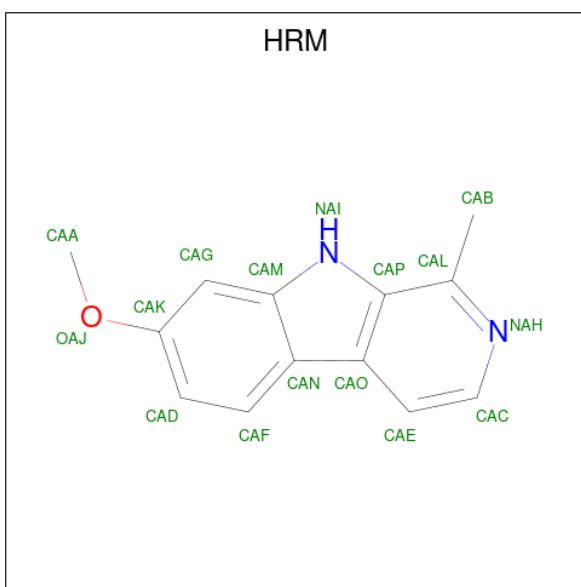
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	0	0	0
			2801	1804	477	502	1	17			
1	B	343	Total	C	N	O	P	S	0	0	0
			2803	1805	480	500	1	17			
1	C	338	Total	C	N	O	P	S	0	0	0
			2773	1787	474	494	1	17			
1	D	341	Total	C	N	O	P	S	0	0	0
			2793	1797	479	499	1	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	123	GLY	-	expression tag	UNP Q13627
A	124	ALA	-	expression tag	UNP Q13627
A	125	SER	-	expression tag	UNP Q13627
B	123	GLY	-	expression tag	UNP Q13627
B	124	ALA	-	expression tag	UNP Q13627
B	125	SER	-	expression tag	UNP Q13627
C	123	GLY	-	expression tag	UNP Q13627
C	124	ALA	-	expression tag	UNP Q13627
C	125	SER	-	expression tag	UNP Q13627
D	123	GLY	-	expression tag	UNP Q13627
D	124	ALA	-	expression tag	UNP Q13627
D	125	SER	-	expression tag	UNP Q13627

- Molecule 2 is 7-METHOXY-1-METHYL-9H-BETA-CARBOLINE (CCD ID: HRM) (formula: C₁₃H₁₂N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 16	C 13	N 2	O 1	0	0
2	B	1	Total 16	C 13	N 2	O 1	0	0
2	C	1	Total 16	C 13	N 2	O 1	0	0
2	D	1	Total 16	C 13	N 2	O 1	0	0

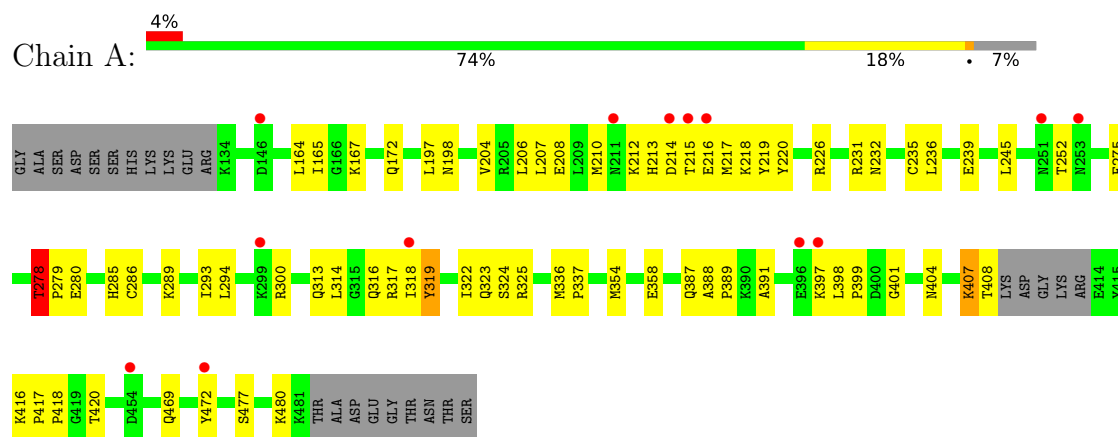
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	6	Total O 6 6	0	0
3	C	6	Total O 6 6	0	0
3	D	7	Total O 7 7	0	0

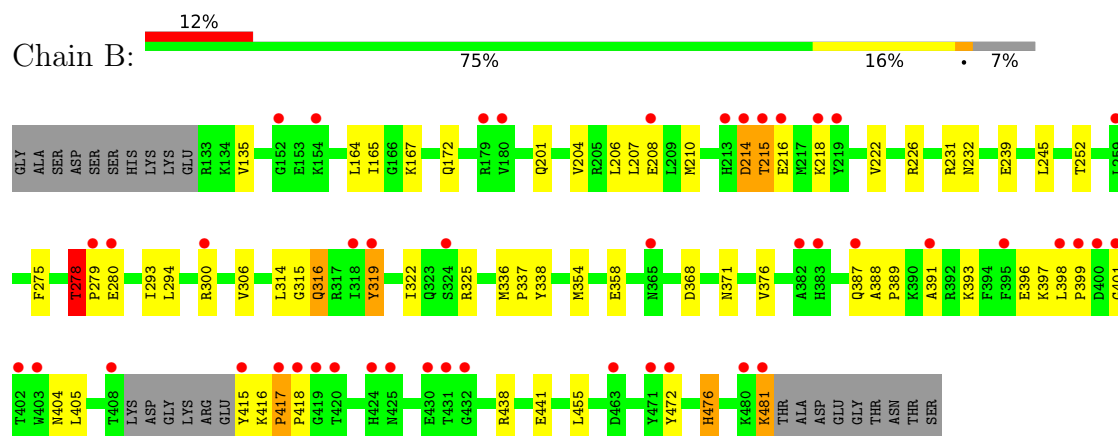
3 Residue-property plots [i](#)

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.

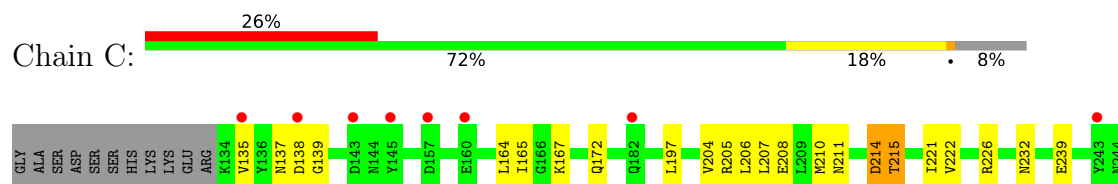
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

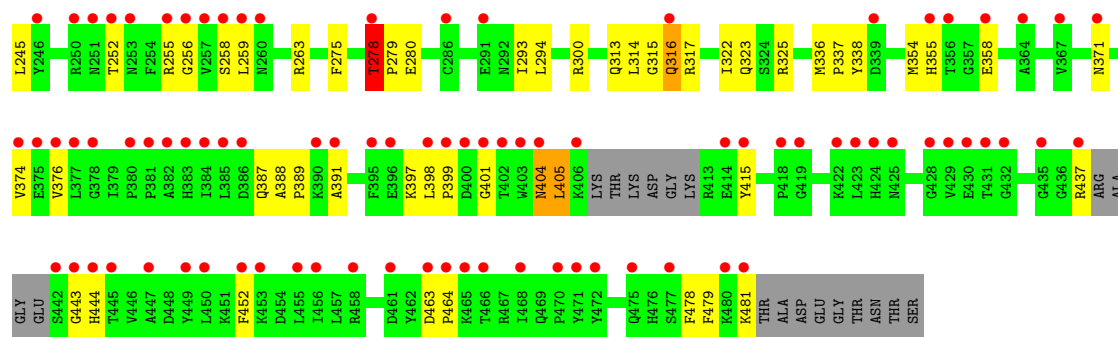


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

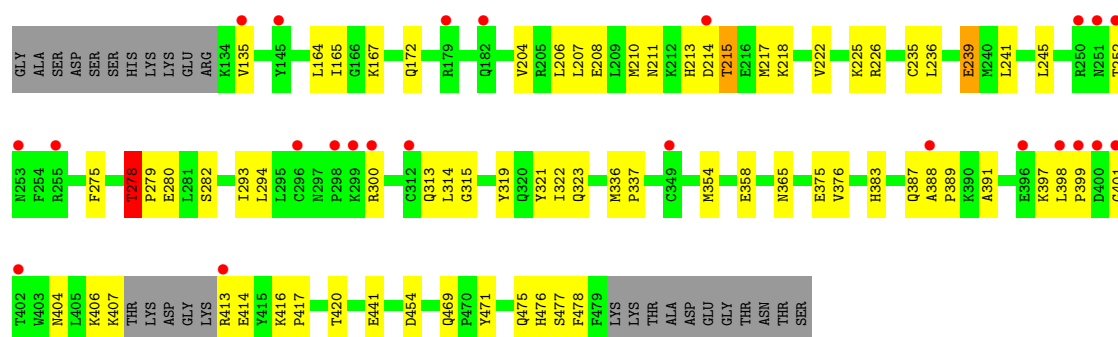


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.58Å 88.14Å 227.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.86 – 2.60 27.86 – 2.61	Depositor EDS
% Data completeness (in resolution range)	85.9 (27.86-2.60) 85.9 (27.86-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.62 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.232 , 0.264 0.232 , 0.264	Depositor DCC
R_{free} test set	2328 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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

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

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	0.63	0/2849	0.97	9/3841 (0.2%)
1	B	0.55	0/2851	0.94	9/3843 (0.2%)
1	C	0.50	0/2820	0.91	6/3800 (0.2%)
1	D	0.57	0/2841	0.93	9/3830 (0.2%)
All	All	0.57	0/11361	0.94	33/15314 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	THR	CA-C-N	6.75	128.28	119.84
1	B	278	THR	C-N-CA	6.75	128.28	119.84
1	A	278	THR	CA-C-N	6.65	128.16	119.84
1	A	278	THR	C-N-CA	6.65	128.16	119.84
1	C	278	THR	CA-C-N	6.64	128.14	119.84
1	C	278	THR	C-N-CA	6.64	128.14	119.84
1	B	417	PRO	CA-C-N	6.57	128.05	119.84
1	B	417	PRO	C-N-CA	6.57	128.05	119.84
1	D	278	THR	CA-C-N	6.49	127.95	119.84
1	D	278	THR	C-N-CA	6.49	127.95	119.84
1	A	252	THR	N-CA-C	-6.45	105.05	113.17
1	D	252	THR	N-CA-C	-6.38	105.13	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	LYS	CA-C-N	6.32	124.27	119.66
1	A	416	LYS	C-N-CA	6.32	124.27	119.66
1	B	252	THR	N-CA-C	-6.19	105.31	112.92
1	D	376	VAL	N-CA-C	6.16	117.11	111.81
1	C	239	GLU	N-CA-C	-6.16	101.81	110.50
1	D	215	THR	N-CA-C	6.08	120.00	110.32
1	D	135	VAL	N-CA-C	6.08	116.37	107.37
1	A	239	GLU	N-CA-C	-6.01	102.02	110.50
1	B	239	GLU	N-CA-C	-5.87	102.36	110.35
1	C	376	VAL	N-CA-C	5.86	116.85	111.81
1	B	376	VAL	N-CA-C	5.78	116.78	111.81
1	C	252	THR	N-CA-C	-5.78	105.82	112.92
1	A	325	ARG	N-CA-C	5.76	118.03	111.11
1	D	239	GLU	N-CA-C	-5.57	102.65	110.50
1	C	325	ARG	N-CA-C	5.45	117.64	111.11
1	B	393	LYS	N-CA-C	-5.26	107.03	113.50
1	A	469	GLN	CA-C-N	5.18	126.31	119.84
1	A	469	GLN	C-N-CA	5.18	126.31	119.84
1	D	469	GLN	CA-C-N	5.08	126.19	119.84
1	D	469	GLN	C-N-CA	5.08	126.19	119.84
1	B	325	ARG	N-CA-C	5.02	117.13	111.11

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	TYR	Sidechain

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	2801	0	2800	55	0
1	B	2803	0	2807	45	0
1	C	2773	0	2776	57	0
1	D	2793	0	2791	58	0
2	A	16	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	0	12	1	0
2	C	16	0	12	1	0
2	D	16	0	12	1	0
3	A	13	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	1	0
3	D	7	0	0	0	0
All	All	11266	0	11222	191	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 9.

All (191) 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:D:215:THR:HG22	1:D:217:MET:H	1.16	1.09
1:A:318:ILE:HG21	1:B:201:GLN:HE22	1.23	1.01
1:A:318:ILE:CG2	1:B:201:GLN:HE22	1.86	0.88
1:B:481:LYS:HD3	1:B:481:LYS:H	1.41	0.86
1:B:275:PHE:O	1:B:278:THR:HG23	1.75	0.85
1:B:245:LEU:HD13	1:B:354:MET:HE2	1.57	0.84
1:D:275:PHE:O	1:D:278:THR:HG23	1.77	0.83
1:C:275:PHE:O	1:C:278:THR:HG23	1.79	0.83
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.62	0.82
1:B:438:ARG:O	1:B:441:GLU:HB2	1.80	0.81
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.61	0.81
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.62	0.80
1:B:316:GLN:H	1:B:316:GLN:HE21	1.26	0.80
1:A:275:PHE:O	1:A:278:THR:HG23	1.79	0.79
1:D:245:LEU:HD13	1:D:354:MET:HE2	1.63	0.78
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.64	0.78
1:A:213:HIS:O	1:A:218:LYS:HD3	1.85	0.76
1:B:481:LYS:HD3	1:B:481:LYS:N	2.00	0.75
1:A:407:LYS:HG3	1:A:408:THR:H	1.50	0.74
1:C:258:SER:HB2	1:C:444:HIS:CE1	2.23	0.73
1:C:317:ARG:HH11	1:C:337:PRO:HA	1.53	0.72
1:C:245:LEU:HD13	1:C:354:MET:HE2	1.72	0.72
1:C:479:PHE:O	1:C:481:LYS:HD3	1.90	0.71
1:B:316:GLN:H	1:B:316:GLN:NE2	1.88	0.70
1:A:204:VAL:O	1:A:208:GLU:HG3	1.92	0.70
1:B:204:VAL:O	1:B:208:GLU:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ILE:HD12	2:D:1:HRM:HAA2	1.76	0.67
1:C:256:GLY:HA3	1:C:355:HIS:O	1.96	0.66
1:C:316:GLN:HA	1:C:316:GLN:OE1	1.95	0.66
1:A:279:PRO:HG3	1:D:337:PRO:HG3	1.78	0.65
1:A:472:TYR:CZ	1:D:383:HIS:HB2	2.32	0.65
1:C:204:VAL:O	1:C:208:GLU:HG3	1.96	0.65
1:C:258:SER:HB2	1:C:444:HIS:HE1	1.62	0.64
1:D:417:PRO:HB2	1:D:420:THR:HG21	1.80	0.64
1:D:471:TYR:CE2	1:D:475:GLN:NE2	2.67	0.62
1:D:204:VAL:O	1:D:208:GLU:HG3	2.00	0.62
1:D:413:ARG:HG2	1:D:413:ARG:HH11	1.65	0.61
1:C:138:ASP:OD2	1:D:365:ASN:HB2	2.00	0.61
1:A:316:GLN:O	1:A:318:ILE:HG13	2.00	0.61
1:C:135:VAL:HG22	1:C:139:GLY:N	2.15	0.61
1:D:208:GLU:O	1:D:211:ASN:HB2	2.00	0.61
1:B:387:GLN:O	1:B:389:PRO:HD3	2.01	0.60
1:C:387:GLN:O	1:C:389:PRO:HD3	2.01	0.60
1:A:207:LEU:HD23	1:A:210:MET:HE3	1.81	0.60
1:D:300:ARG:HH11	1:D:300:ARG:HG3	1.66	0.60
1:A:387:GLN:O	1:A:389:PRO:HD3	2.02	0.60
1:C:317:ARG:HH11	1:C:337:PRO:CA	2.15	0.59
1:A:217:MET:HB3	1:A:275:PHE:HB2	1.84	0.59
1:D:406:LYS:O	1:D:406:LYS:HG2	2.02	0.59
1:A:472:TYR:CE1	1:D:383:HIS:HB2	2.37	0.59
1:C:207:LEU:HD23	1:C:210:MET:HE3	1.85	0.59
1:C:205:ARG:HH12	1:C:313:GLN:NE2	2.01	0.59
1:D:387:GLN:O	1:D:389:PRO:HD3	2.02	0.59
1:B:336:MET:HB3	1:B:337:PRO:CD	2.33	0.59
1:D:207:LEU:HD23	1:D:210:MET:HE3	1.84	0.58
1:C:300:ARG:HG3	1:C:300:ARG:HH11	1.67	0.58
1:A:206:LEU:O	1:A:210:MET:HG3	2.04	0.57
1:B:300:ARG:HH11	1:B:300:ARG:HG3	1.70	0.57
1:A:245:LEU:HD13	1:A:354:MET:HE2	1.87	0.57
1:C:336:MET:HB3	1:C:337:PRO:CD	2.34	0.57
1:D:336:MET:HB3	1:D:337:PRO:CD	2.35	0.56
1:A:198:ASN:HD21	1:B:319:TYR:HE1	1.53	0.56
1:B:207:LEU:HD23	1:B:210:MET:HE3	1.86	0.56
1:A:197:LEU:HD23	1:B:319:TYR:HD1	1.71	0.56
1:C:255:ARG:HD3	1:C:437:ARG:NE	2.20	0.56
1:D:213:HIS:O	1:D:218:LYS:HD3	2.06	0.56
1:A:300:ARG:HH11	1:A:300:ARG:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:GLN:O	1:A:318:ILE:N	2.39	0.55
1:A:318:ILE:CG2	1:B:201:GLN:NE2	2.65	0.55
1:B:165:ILE:HD12	2:B:1:HRM:HAA2	1.87	0.55
1:A:336:MET:HB3	1:A:337:PRO:CD	2.37	0.55
1:B:206:LEU:O	1:B:210:MET:HG3	2.07	0.54
1:D:375:GLU:OE2	1:D:416:LYS:HG3	2.08	0.54
1:A:472:TYR:OH	1:D:383:HIS:HB2	2.08	0.54
1:D:398:LEU:HB3	1:D:399:PRO:HD2	1.89	0.54
1:B:314:LEU:O	1:C:315:GLY:HA3	2.07	0.53
1:D:417:PRO:HB2	1:D:420:THR:CG2	2.37	0.53
1:D:398:LEU:HD11	1:D:404:ASN:ND2	2.25	0.52
1:A:472:TYR:CZ	1:D:387:GLN:NE2	2.77	0.52
1:C:197:LEU:HD23	1:D:319:TYR:CD1	2.44	0.52
1:A:318:ILE:HB	1:A:319:TYR:CD1	2.45	0.52
1:B:316:GLN:HE21	1:B:316:GLN:N	2.03	0.52
1:B:397:LYS:HE2	1:B:401:GLY:HA2	1.92	0.52
1:C:214:ASP:O	1:C:215:THR:O	2.28	0.51
1:C:398:LEU:HB3	1:C:399:PRO:HD2	1.91	0.51
1:D:406:LYS:C	1:D:407:LYS:HG2	2.35	0.51
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.91	0.51
1:D:215:THR:HG22	1:D:217:MET:N	2.02	0.51
1:A:398:LEU:HB3	1:A:399:PRO:HD2	1.93	0.50
1:C:138:ASP:CG	1:D:365:ASN:HB2	2.37	0.50
1:A:397:LYS:HE2	1:A:401:GLY:HA2	1.93	0.50
1:D:397:LYS:HE2	1:D:401:GLY:HA2	1.93	0.49
1:C:397:LYS:HE2	1:C:401:GLY:HA2	1.93	0.49
1:A:314:LEU:O	1:D:315:GLY:HA2	2.12	0.49
1:B:396:GLU:HG2	1:B:404:ASN:O	2.12	0.49
1:D:211:ASN:C	1:D:213:HIS:H	2.21	0.49
1:B:336:MET:HB3	1:B:337:PRO:HD2	1.95	0.48
1:A:318:ILE:HB	1:A:319:TYR:CE1	2.47	0.48
1:C:232:ASN:ND2	1:D:321:PTR:HB3	2.29	0.48
1:A:417:PRO:HB2	1:A:420:THR:HG21	1.95	0.48
1:A:216:GLU:HA	1:A:219:TYR:CD2	2.49	0.48
1:D:206:LEU:O	1:D:210:MET:HG3	2.13	0.48
1:C:371:ASN:HB3	1:C:415:TYR:CD2	2.49	0.48
1:C:206:LEU:O	1:C:210:MET:HG3	2.14	0.47
1:D:300:ARG:HG3	1:D:300:ARG:NH1	2.29	0.47
1:A:164:LEU:HD11	1:A:172:GLN:HB3	1.96	0.47
1:C:245:LEU:HB3	1:C:354:MET:CE	2.43	0.47
1:C:314:LEU:HG	1:C:315:GLY:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:LYS:HD3	1:C:481:LYS:N	2.29	0.47
1:A:210:MET:C	1:A:212:LYS:H	2.23	0.47
1:B:455:LEU:HD13	1:B:476:HIS:CD2	2.50	0.47
1:A:417:PRO:HB2	1:A:420:THR:CG2	2.45	0.46
1:D:293:ILE:C	1:D:294:LEU:HD12	2.40	0.46
1:A:316:GLN:HE22	1:D:282:SER:HB2	1.80	0.46
1:A:398:LEU:HD11	1:A:404:ASN:OD1	2.15	0.46
1:A:235:CYS:C	1:A:236:LEU:HD23	2.40	0.46
1:A:472:TYR:HH	1:D:383:HIS:C	2.23	0.46
1:C:263:ARG:HD3	1:C:479:PHE:HA	1.97	0.46
1:A:322:ILE:O	1:A:323:GLN:HB2	2.16	0.46
1:C:137:ASN:O	1:C:138:ASP:HB2	2.16	0.46
1:C:263:ARG:NE	1:C:478:PHE:O	2.46	0.46
1:D:164:LEU:HD11	1:D:172:GLN:HB3	1.98	0.46
1:C:374:VAL:HG11	1:C:405:LEU:HD21	1.99	0.45
1:A:280:GLU:H	1:A:280:GLU:CD	2.22	0.45
1:C:463:ASP:HA	1:C:464:PRO:HD2	1.88	0.45
1:C:300:ARG:HG3	1:C:300:ARG:NH1	2.29	0.45
1:C:443:GLY:C	1:C:444:HIS:HD1	2.24	0.45
1:D:279:PRO:HB2	1:D:280:GLU:OE1	2.16	0.45
1:C:255:ARG:HD3	1:C:437:ARG:CD	2.46	0.45
1:D:214:ASP:C	1:D:214:ASP:OD2	2.60	0.45
1:B:416:LYS:O	1:B:417:PRO:C	2.60	0.45
1:A:313:GLN:O	1:A:314:LEU:C	2.59	0.45
1:B:300:ARG:HG3	1:B:300:ARG:NH1	2.32	0.45
1:C:336:MET:HB3	1:C:337:PRO:HD2	1.98	0.45
1:A:336:MET:HB3	1:A:337:PRO:HD2	1.99	0.44
1:C:279:PRO:HB2	1:C:280:GLU:OE1	2.17	0.44
1:B:337:PRO:HG3	1:C:279:PRO:HG3	1.99	0.44
1:C:322:ILE:O	1:C:323:GLN:HB2	2.17	0.44
1:D:336:MET:HB3	1:D:337:PRO:HD2	1.98	0.44
1:C:164:LEU:HD11	1:C:172:GLN:HB3	1.98	0.44
1:B:417:PRO:HA	1:B:418:PRO:HD3	1.79	0.44
1:D:413:ARG:HG2	1:D:413:ARG:NH1	2.33	0.44
1:A:231:ARG:O	1:A:232:ASN:HB2	2.18	0.44
1:B:214:ASP:CG	1:B:215:THR:N	2.75	0.44
1:B:164:LEU:HD11	1:B:172:GLN:HB3	2.00	0.43
1:A:279:PRO:HB2	1:A:280:GLU:OE1	2.18	0.43
1:A:300:ARG:HG3	1:A:300:ARG:NH1	2.32	0.43
1:B:278:THR:HA	1:B:279:PRO:HD3	1.84	0.43
1:C:293:ILE:C	1:C:294:LEU:HD12	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:VAL:CG2	1:C:139:GLY:N	2.80	0.43
1:D:211:ASN:HD22	1:D:211:ASN:HA	1.60	0.43
1:D:454:ASP:OD2	1:D:476:HIS:NE2	2.43	0.43
1:A:216:GLU:HG3	1:A:219:TYR:CD2	2.53	0.43
1:A:289:LYS:HD3	1:A:324:SER:OG	2.18	0.43
1:A:472:TYR:OH	1:D:383:HIS:O	2.33	0.43
1:A:477:SER:HA	1:A:480:LYS:HB2	2.00	0.43
1:B:279:PRO:HB3	1:C:317:ARG:CZ	2.49	0.43
1:B:279:PRO:HB2	1:B:280:GLU:OE1	2.18	0.43
1:A:278:THR:HA	1:A:279:PRO:HD3	1.79	0.43
1:B:368:ASP:HA	1:B:415:TYR:OH	2.18	0.43
1:D:280:GLU:H	1:D:280:GLU:CD	2.26	0.42
1:C:404:ASN:O	1:C:405:LEU:O	2.36	0.42
1:A:285:HIS:O	1:A:286:CYS:HB2	2.18	0.42
1:C:165:ILE:HD12	2:C:1:HRM:HAA2	2.01	0.42
1:D:477:SER:O	1:D:478:PHE:C	2.63	0.42
1:A:293:ILE:C	1:A:294:LEU:HD12	2.44	0.42
1:D:211:ASN:C	1:D:213:HIS:N	2.78	0.42
1:B:405:LEU:HD11	1:B:418:PRO:HG3	2.00	0.42
1:D:406:LYS:O	1:D:407:LYS:C	2.63	0.42
1:C:197:LEU:HD23	1:D:319:TYR:HD1	1.83	0.42
1:B:371:ASN:HB3	1:B:415:TYR:CE1	2.55	0.41
1:B:231:ARG:O	1:B:232:ASN:HB2	2.20	0.41
1:C:259:LEU:HD11	1:C:452:PHE:CG	2.55	0.41
1:A:280:GLU:OE1	1:A:280:GLU:N	2.43	0.41
1:B:472:TYR:OH	1:C:387:GLN:NE2	2.53	0.41
1:C:167:LYS:HD3	3:C:8:HOH:O	2.19	0.41
1:D:322:ILE:O	1:D:323:GLN:HB2	2.20	0.41
1:D:280:GLU:OE1	1:D:280:GLU:N	2.46	0.41
1:B:293:ILE:C	1:B:294:LEU:HD12	2.46	0.41
1:C:280:GLU:H	1:C:280:GLU:CD	2.26	0.41
1:D:225:LYS:HE2	1:D:239:GLU:HA	2.03	0.41
1:D:313:GLN:O	1:D:314:LEU:C	2.63	0.41
1:B:222:VAL:HB	1:B:306:VAL:HG12	2.01	0.41
1:D:235:CYS:C	1:D:236:LEU:HD23	2.46	0.41
1:D:222:VAL:HG23	1:D:241:LEU:HD11	2.02	0.40
1:A:407:LYS:CG	1:A:408:THR:H	2.20	0.40
1:C:221:ILE:O	1:C:222:VAL:C	2.63	0.40
1:A:165:ILE:HD12	2:A:1:HRM:HAA2	2.04	0.40
1:B:315:GLY:HA2	1:C:314:LEU:O	2.21	0.40
1:B:322:ILE:HD13	1:B:338:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ILE:HD13	1:C:338:TYR:CZ	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	338/368 (92%)	314 (93%)	20 (6%)	4 (1%)	10	23
1	B	338/368 (92%)	309 (91%)	24 (7%)	5 (2%)	8	18
1	C	331/368 (90%)	304 (92%)	25 (8%)	2 (1%)	21	42
1	D	336/368 (91%)	314 (94%)	22 (6%)	0	100	100
All	All	1343/1472 (91%)	1241 (92%)	91 (7%)	11 (1%)	16	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	THR
1	A	317	ARG
1	A	407	LYS
1	B	214	ASP
1	B	215	THR
1	C	215	THR
1	C	405	LEU
1	B	218	LYS
1	A	214	ASP
1	B	216	GLU
1	B	476	HIS

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	302/324 (93%)	296 (98%)	6 (2%)	48	74
1	B	302/324 (93%)	294 (97%)	8 (3%)	40	68
1	C	300/324 (93%)	293 (98%)	7 (2%)	44	71
1	D	301/324 (93%)	295 (98%)	6 (2%)	48	74
All	All	1205/1296 (93%)	1178 (98%)	27 (2%)	45	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
1	A	226	ARG
1	A	278	THR
1	A	319	TYR
1	A	358	GLU
1	A	418	PRO
1	B	135	VAL
1	B	167	LYS
1	B	226	ARG
1	B	278	THR
1	B	316	GLN
1	B	319	TYR
1	B	358	GLU
1	B	481	LYS
1	C	211	ASN
1	C	214	ASP
1	C	226	ARG
1	C	278	THR
1	C	316	GLN
1	C	358	GLU
1	C	404	ASN
1	D	167	LYS
1	D	226	ARG
1	D	278	THR

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Mol	Chain	Res	Type
1	D	358	GLU
1	D	414	GLU
1	D	441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	182	GLN
1	A	198	ASN
1	A	201	GLN
1	A	211	ASN
1	A	223	HIS
1	A	232	ASN
1	A	251	ASN
1	A	316	GLN
1	A	320	GLN
1	A	425	ASN
1	B	151	ASN
1	B	182	GLN
1	B	198	ASN
1	B	201	GLN
1	B	223	HIS
1	B	232	ASN
1	B	251	ASN
1	B	316	GLN
1	B	387	GLN
1	B	404	ASN
1	B	425	ASN
1	C	151	ASN
1	C	182	GLN
1	C	198	ASN
1	C	211	ASN
1	C	213	HIS
1	C	232	ASN
1	C	251	ASN
1	C	313	GLN
1	C	387	GLN
1	C	425	ASN
1	C	475	GLN
1	D	151	ASN
1	D	182	GLN

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Mol	Chain	Res	Type
1	D	198	ASN
1	D	211	ASN
1	D	213	HIS
1	D	251	ASN
1	D	387	GLN
1	D	404	ASN
1	D	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PTR	C	321	1	15,16,17	1.22	0	17,22,24	0.64	0
1	PTR	A	321	1	15,16,17	1.10	0	17,22,24	0.65	0
1	PTR	D	321	1	15,16,17	1.09	0	17,22,24	0.72	0
1	PTR	B	321	1	15,16,17	1.04	0	17,22,24	0.69	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	321	1	-	2/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	D	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	321	PTR	CA-CB-CG-CD2
1	C	321	PTR	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HRM	C	1	-	17,18,18	2.58	9 (52%)	22,26,26	1.93	6 (27%)
2	HRM	D	1	-	17,18,18	2.58	10 (58%)	22,26,26	1.88	5 (22%)
2	HRM	B	1	-	17,18,18	2.37	9 (52%)	22,26,26	1.78	5 (22%)
2	HRM	A	1	-	17,18,18	2.50	10 (58%)	22,26,26	1.81	4 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HRM	C	1	-	-	0/2/2/2	0/3/3/3
2	HRM	D	1	-	-	0/2/2/2	0/3/3/3
2	HRM	B	1	-	-	0/2/2/2	0/3/3/3
2	HRM	A	1	-	-	0/2/2/2	0/3/3/3

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	HRM	CAD-CAK	4.63	1.47	1.38
2	D	1	HRM	CAF-CAN	4.60	1.47	1.40
2	A	1	HRM	CAM-NAI	-4.28	1.31	1.38
2	C	1	HRM	CAG-CAK	4.23	1.46	1.39
2	C	1	HRM	CAF-CAN	4.18	1.46	1.40
2	A	1	HRM	CAF-CAN	3.58	1.45	1.40
2	B	1	HRM	CAN-CAO	-3.55	1.37	1.46
2	A	1	HRM	CAN-CAO	-3.48	1.37	1.46
2	B	1	HRM	CAD-CAK	3.44	1.45	1.38
2	C	1	HRM	CAN-CAO	-3.39	1.38	1.46
2	D	1	HRM	CAG-CAK	3.38	1.44	1.39
2	D	1	HRM	CAD-CAF	3.37	1.44	1.38
2	A	1	HRM	CAD-CAF	3.24	1.44	1.38
2	B	1	HRM	CAG-CAK	3.11	1.44	1.39
2	C	1	HRM	CAL-NAH	3.05	1.39	1.33
2	A	1	HRM	CAP-NAI	-3.04	1.34	1.38
2	C	1	HRM	CAD-CAF	2.99	1.43	1.38
2	B	1	HRM	CAF-CAN	2.91	1.44	1.40
2	C	1	HRM	CAE-CAO	2.85	1.44	1.40
2	D	1	HRM	CAN-CAO	-2.83	1.39	1.46
2	B	1	HRM	CAL-NAH	2.81	1.38	1.33
2	B	1	HRM	CAE-CAO	2.81	1.44	1.40
2	D	1	HRM	CAO-CAP	2.79	1.45	1.41
2	C	1	HRM	CAD-CAK	2.73	1.43	1.38
2	A	1	HRM	CAD-CAK	2.70	1.43	1.38
2	C	1	HRM	CAP-NAI	-2.65	1.34	1.38
2	A	1	HRM	CAL-NAH	2.63	1.38	1.33
2	B	1	HRM	CAC-NAH	2.43	1.39	1.34
2	A	1	HRM	OAJ-CAA	2.36	1.49	1.42
2	B	1	HRM	CAD-CAF	2.28	1.42	1.38
2	B	1	HRM	CAO-CAP	2.22	1.44	1.41
2	C	1	HRM	CAO-CAP	2.22	1.44	1.41
2	D	1	HRM	CAM-NAI	-2.19	1.34	1.38
2	A	1	HRM	CAG-CAK	2.11	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	HRM	CAC-NAH	2.09	1.39	1.34
2	A	1	HRM	CAE-CAO	2.07	1.43	1.40
2	D	1	HRM	OAJ-CAA	2.04	1.48	1.42
2	D	1	HRM	CAE-CAO	2.01	1.43	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	HRM	CAC-NAH-CAL	4.84	123.88	118.35
2	D	1	HRM	CAC-NAH-CAL	4.80	123.83	118.35
2	A	1	HRM	CAC-NAH-CAL	4.59	123.59	118.35
2	B	1	HRM	CAC-NAH-CAL	4.39	123.36	118.35
2	A	1	HRM	CAE-CAC-NAH	-4.03	119.03	123.97
2	C	1	HRM	CAE-CAC-NAH	-3.93	119.16	123.97
2	D	1	HRM	CAF-CAN-CAM	3.79	123.25	119.07
2	C	1	HRM	CAF-CAN-CAM	3.77	123.22	119.07
2	B	1	HRM	CAF-CAN-CAM	3.76	123.22	119.07
2	B	1	HRM	CAE-CAC-NAH	-3.61	119.55	123.97
2	A	1	HRM	CAF-CAN-CAM	3.53	122.97	119.07
2	D	1	HRM	CAE-CAC-NAH	-3.43	119.77	123.97
2	C	1	HRM	CAG-CAM-CAN	-2.84	118.94	122.07
2	B	1	HRM	CAG-CAM-CAN	-2.48	119.33	122.07
2	B	1	HRM	CAO-CAP-NAI	-2.30	106.99	109.29
2	D	1	HRM	CAG-CAM-CAN	-2.28	119.55	122.07
2	D	1	HRM	CAO-CAP-NAI	-2.23	107.06	109.29
2	C	1	HRM	CAO-CAP-NAI	-2.20	107.09	109.29
2	A	1	HRM	CAO-CAP-NAI	-2.03	107.25	109.29
2	C	1	HRM	CAF-CAD-CAK	-2.01	117.44	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	HRM	1	0
2	D	1	HRM	1	0
2	B	1	HRM	1	0
2	A	1	HRM	1	0

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	342/368 (92%)	0.10	13 (3%) 44 38	10, 30, 59, 72	2 (0%)
1	B	342/368 (92%)	0.79	46 (13%) 7 5	15, 46, 83, 104	2 (0%)
1	C	337/368 (91%)	1.34	94 (27%) 1 1	21, 60, 97, 118	2 (0%)
1	D	340/368 (92%)	0.48	24 (7%) 22 17	14, 42, 67, 86	2 (0%)
All	All	1361/1472 (92%)	0.67	177 (13%) 7 5	10, 44, 86, 118	8 (0%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	GLY	7.1
1	C	402	THR	6.3
1	C	419	GLY	5.5
1	C	403	TRP	5.4
1	B	402	THR	5.4
1	C	256	GLY	5.2
1	B	399	PRO	5.2
1	C	253	ASN	5.0
1	C	251	ASN	4.9
1	C	377	LEU	4.7
1	C	143	ASP	4.7
1	C	447	ALA	4.6
1	B	401	GLY	4.4
1	B	218	LYS	4.4
1	C	252	THR	4.3
1	C	414	GLU	4.3
1	C	258	SER	4.1
1	C	381	PRO	4.1
1	C	398	LEU	4.1
1	C	399	PRO	4.0
1	C	160	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	419	GLY	3.9
1	C	378	GLY	3.9
1	B	154	LYS	3.8
1	D	401	GLY	3.8
1	C	383	HIS	3.7
1	B	398	LEU	3.6
1	B	425	ASN	3.6
1	B	214	ASP	3.6
1	A	472	TYR	3.6
1	C	442	SER	3.6
1	C	278	THR	3.5
1	C	286	CYS	3.4
1	C	250	ARG	3.4
1	C	472	TYR	3.3
1	C	435	GLY	3.3
1	C	135	VAL	3.3
1	C	423	LEU	3.3
1	D	300	ARG	3.3
1	C	443	GLY	3.3
1	B	463	ASP	3.3
1	C	255	ARG	3.3
1	C	466	THR	3.3
1	C	316	GLN	3.3
1	C	415	TYR	3.2
1	C	471	TYR	3.2
1	D	298	PRO	3.2
1	A	253	ASN	3.2
1	C	477	SER	3.2
1	B	213	HIS	3.1
1	D	402	THR	3.0
1	B	472	TYR	3.0
1	C	456	ILE	3.0
1	C	182	GLN	3.0
1	C	390	LYS	2.9
1	C	418	PRO	2.9
1	C	382	ALA	2.9
1	D	250	ARG	2.9
1	D	398	LEU	2.9
1	B	180	VAL	2.9
1	A	318	ILE	2.9
1	C	422	LYS	2.9
1	C	458	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	324	SER	2.8
1	C	465	LYS	2.8
1	C	481	LYS	2.8
1	C	371	ASN	2.8
1	B	382	ALA	2.8
1	B	179	ARG	2.8
1	A	251	ASN	2.8
1	D	214	ASP	2.8
1	C	367	VAL	2.8
1	D	296	CYS	2.7
1	D	399	PRO	2.7
1	B	408	THR	2.7
1	D	252	THR	2.7
1	C	260	ASN	2.7
1	C	475	GLN	2.7
1	B	300	ARG	2.7
1	B	418	PRO	2.7
1	C	400	ASP	2.7
1	A	396	GLU	2.6
1	C	396	GLU	2.6
1	C	374	VAL	2.6
1	C	450	LEU	2.6
1	D	413	ARG	2.6
1	C	391	ALA	2.6
1	B	400	ASP	2.6
1	C	449	TYR	2.6
1	D	145	TYR	2.6
1	B	417	PRO	2.6
1	C	364	ALA	2.6
1	B	215	THR	2.6
1	D	299	LYS	2.6
1	C	464	PRO	2.6
1	B	403	TRP	2.5
1	C	339	ASP	2.5
1	C	145	TYR	2.5
1	C	470	PRO	2.5
1	D	253	ASN	2.5
1	B	424	HIS	2.5
1	C	432	GLY	2.5
1	A	454	ASP	2.5
1	B	471	TYR	2.5
1	C	431	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	365	ASN	2.4
1	C	430	GLU	2.4
1	B	420	THR	2.4
1	C	424	HIS	2.4
1	B	219	TYR	2.4
1	C	452	PHE	2.4
1	A	146	ASP	2.4
1	C	461	ASP	2.4
1	B	480	LYS	2.4
1	D	179	ARG	2.4
1	C	384	ILE	2.4
1	D	396	GLU	2.4
1	C	428	GLY	2.4
1	B	391	ALA	2.4
1	C	395	PHE	2.4
1	C	385	LEU	2.3
1	A	216	GLU	2.3
1	B	280	GLU	2.3
1	C	444	HIS	2.3
1	D	251	ASN	2.3
1	D	400	ASP	2.3
1	C	355	HIS	2.3
1	A	215	THR	2.3
1	C	453	LYS	2.3
1	C	480	LYS	2.3
1	C	138	ASP	2.3
1	D	255	ARG	2.3
1	D	182	GLN	2.3
1	D	135	VAL	2.3
1	A	211	ASN	2.3
1	C	437	ARG	2.3
1	B	152	GLY	2.3
1	C	455	LEU	2.3
1	B	395	PHE	2.3
1	C	246	TYR	2.2
1	C	463	ASP	2.2
1	B	208	GLU	2.2
1	C	356	THR	2.2
1	B	319	TYR	2.2
1	B	432	GLY	2.2
1	C	386	ASP	2.2
1	B	216	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	431	THR	2.2
1	B	279	PRO	2.2
1	B	387	GLN	2.2
1	C	259	LEU	2.2
1	C	429	VAL	2.2
1	B	318	ILE	2.2
1	D	388	ALA	2.2
1	C	358	GLU	2.2
1	A	397	LYS	2.1
1	C	404	ASN	2.1
1	C	157	ASP	2.1
1	A	214	ASP	2.1
1	C	376	VAL	2.1
1	A	299	LYS	2.1
1	C	380	PRO	2.1
1	B	383	HIS	2.1
1	C	257	VAL	2.1
1	B	430	GLU	2.1
1	C	291	GLU	2.1
1	B	259	LEU	2.1
1	D	312	CYS	2.1
1	D	349	CYS	2.1
1	C	406	LYS	2.0
1	C	425	ASN	2.0
1	C	468	ILE	2.0
1	B	415	TYR	2.0
1	C	243	TYR	2.0
1	C	375	GLU	2.0
1	B	481	LYS	2.0
1	C	445	THR	2.0

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

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(Å ²)	Q<0.9
1	PTR	C	321	16/17	0.91	0.11	31,42,44,46	0
1	PTR	B	321	16/17	0.95	0.10	38,45,46,50	0
1	PTR	D	321	16/17	0.97	0.08	26,28,31,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	PTR	A	321	16/17	0.98	0.06	16,22,29,36	0

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
2	HRM	C	1	16/16	0.96	0.07	27,33,40,42	0
2	HRM	D	1	16/16	0.96	0.05	24,31,34,35	0
2	HRM	B	1	16/16	0.97	0.05	15,20,26,30	0
2	HRM	A	1	16/16	0.98	0.05	5,11,16,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.