



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:26 pm BST

PDB ID : 3ANR  
Title : human DYRK1A/harmine complex  
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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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

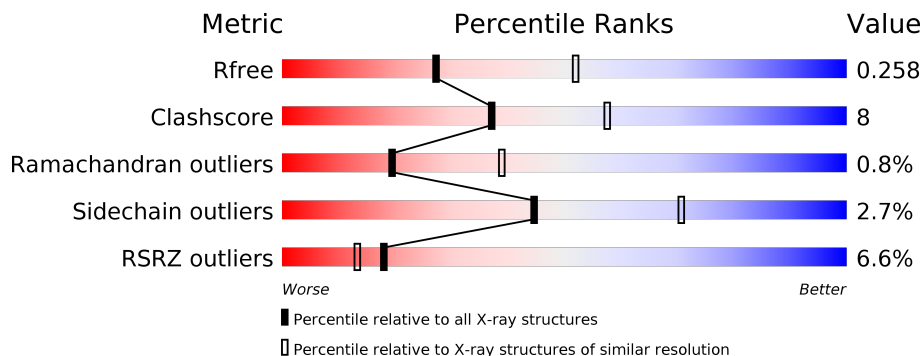
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	
1	B	368	
1	C	368	
1	D	368	

## 2 Entry composition [i](#)

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.

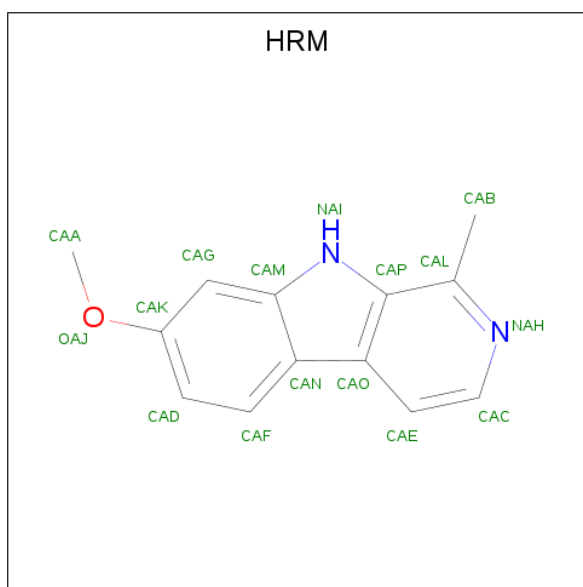
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

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

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 (three-letter code: HRM) (formula: C<sub>13</sub>H<sub>12</sub>N<sub>2</sub>O).



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

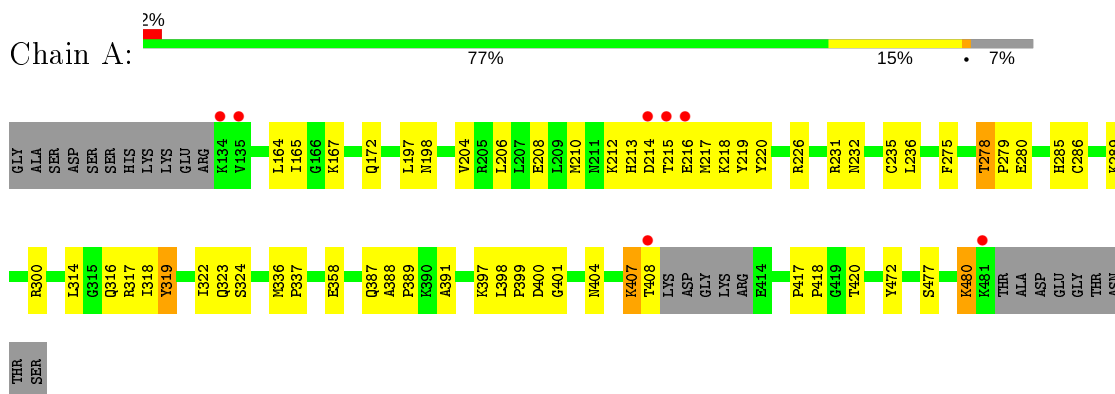
- Molecule 3 is water.

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

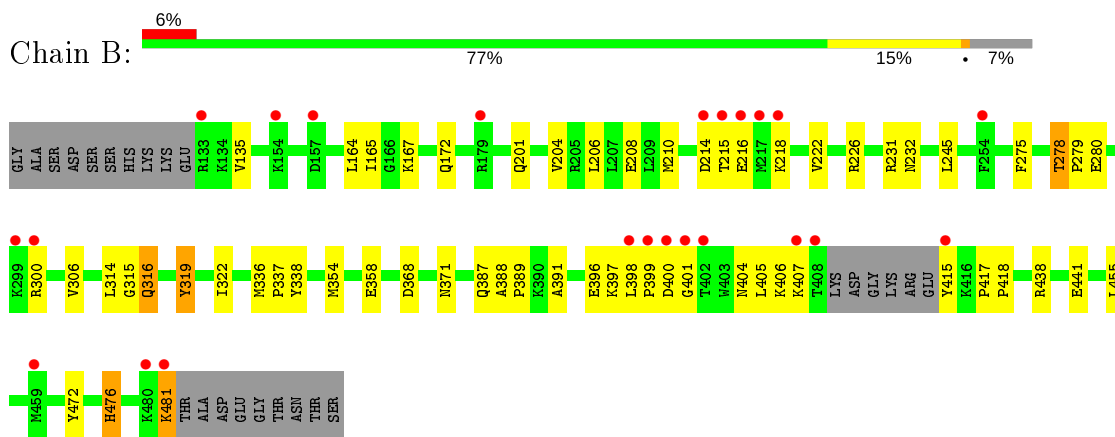
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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.

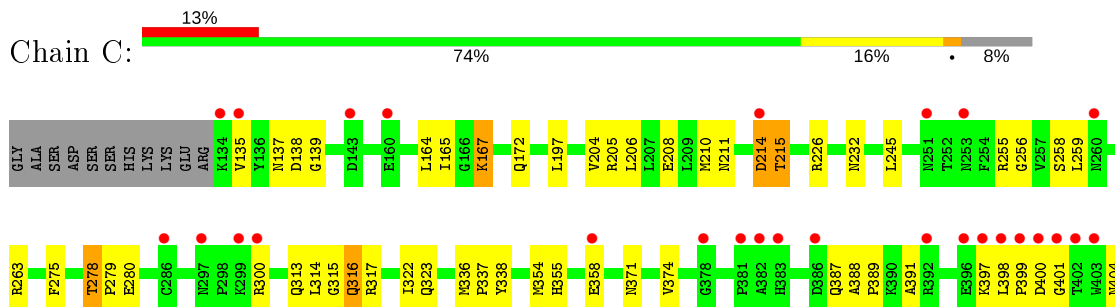
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

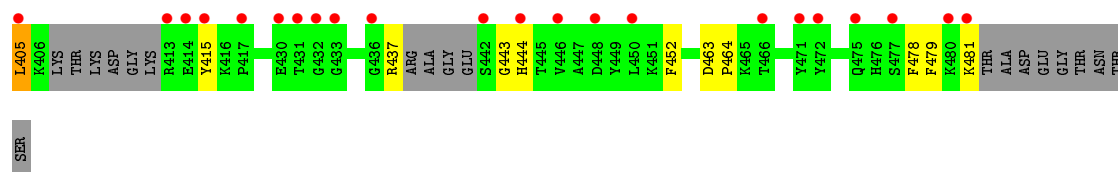


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

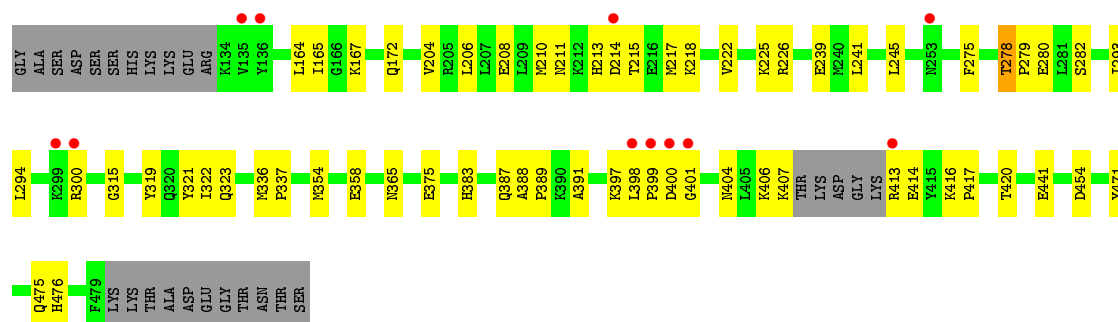
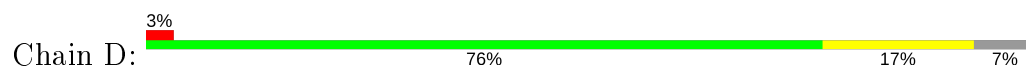


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





- 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, $\alpha$ , $\beta$ , $\gamma$	87.58Å 88.14Å 227.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.86 – 2.60 27.85 – 2.61	Depositor EDS
% Data completeness (in resolution range)	85.9 (27.86-2.60) 86.0 (27.85-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	15.62 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.232 , 0.264 0.223 , 0.258	Depositor DCC
$R_{free}$ test set	2328 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtrriage
Anisotropy	0.420	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.035 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11266	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: HRM, PTR

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	0.53	0/2849	0.65	0/3841
1	B	0.46	0/2851	0.63	0/3843
1	C	0.44	0/2820	0.61	0/3800
1	D	0.48	0/2841	0.62	0/3830
All	All	0.48	0/11361	0.63	0/15314

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.

There are no bond angle outliers.

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

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	51	0
1	B	2803	0	2807	43	0
1	C	2773	0	2776	53	0
1	D	2793	0	2791	52	0
2	A	16	0	12	1	0
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	175	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 8.

All (175) 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:H	1:B:481:LYS:HD3	1.41	0.86
1:B:275:PHE:O	1:B:278:THR:HG23	1.75	0.85
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:HE21	1:B:316:GLN:H	1.26	0.80
1:A:275:PHE:O	1:A:278:THR:HG23	1.79	0.79
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:N	1:B:481:LYS:HD3	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:VAL:O	1:B:208:GLU:HG3	1.93	0.69
1:D:165:ILE:HD12	2:D:1:HRM:HAA2	1.76	0.67
1:C:245:LEU:HB3	1:C:354:MET:HE1	1.77	0.67
1:C:256:GLY:HA3	1:C:355:HIS:O	1.96	0.66
1:C:316:GLN:OE1	1:C:316:GLN:HA	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:HH11	1:D:413:ARG:HG2	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: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:HG2	1:D:406:LYS:O	2.02	0.59
1:A:472:TYR:CE1	1:D:383:HIS:HB2	2.37	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:C:300:ARG:HH11	1:C:300:ARG:HG3	1.67	0.58
1:A:206:LEU:O	1:A:210:MET:HG3	2.04	0.57
1:B:300:ARG:HG3	1:B:300:ARG:HH11	1.70	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:245:LEU:HB3	1:B:354:MET:HE1	1.91	0.53
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: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:D:245:LEU:HD13	1:D:354:MET:HE2	1.94	0.50
1:A:398:LEU:HB3	1:A:399:PRO:HD2	1.93	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: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:314:LEU:HG	1:C:315:GLY:N	2.30	0.47
1:C:245:LEU:HB3	1:C:354:MET:CE	2.43	0.47
1:C:481:LYS:N	1:C:481:LYS:HD3	2.29	0.47
1:D:406:LYS:C	1:D:407:LYS:HG2	2.35	0.47
1:B:455:LEU:HD13	1:B:476:HIS:CD2	2.50	0.47
1:D:245:LEU:HB3	1:D:354:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:PRO:HB2	1:A:420:THR:CG2	2.45	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: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:C:463:ASP:HA	1:C:464:PRO:HD2	1.88	0.45
1:C:300:ARG:NH1	1:C:300:ARG:HG3	2.29	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: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:138:ASP:CG	1:D:365:ASN:HB2	2.37	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:NH1	1:D:413:ARG:HG2	2.33	0.44
1:A:231:ARG:O	1:A:232:ASN:HB2	2.18	0.44
1:B:245:LEU:HD13	1:B:354:MET:CE	2.48	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:135:VAL:CG2	1:C:139:GLY:N	2.80	0.43
1:D:211:ASN:HA	1:D:211:ASN:HD22	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:D:211:ASN:C	1:D:213:HIS:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:HA	1:B:415:TYR:OH	2.18	0.43
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:B:231:ARG:O	1:B:232:ASN:HB2	2.20	0.42
1:A:210:MET:C	1:A:212:LYS:H	2.23	0.42
1:A:235:CYS:C	1:A:236:LEU:HD23	2.40	0.42
1:A:472:TYR:HH	1:D:383:HIS:C	2.22	0.42
1:B:405:LEU:HD11	1:B:418:PRO:HG3	2.00	0.42
1:D:293:ILE:C	1:D:294:LEU:HD12	2.40	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: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:C:167:LYS:HD3	3:C:8:HOH:O	2.19	0.41
1:B:472:TYR:OH	1:C:387:GLN:NE2	2.53	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:D:225:LYS:HE2	1:D:239:GLU:HA	2.03	0.41
1:B:222:VAL:HB	1:B:306:VAL:HG12	2.01	0.41
1:C:443:GLY:C	1:C:444:HIS:HD1	2.24	0.40
1:D:222:VAL:HG23	1:D:241:LEU:HD11	2.02	0.40
1:A:280:GLU:CD	1:A:280:GLU:H	2.22	0.40
1:A:407:LYS:CG	1:A:408:THR:H	2.20	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
1:B:406:LYS:CG	1:B:407:LYS:N	2.85	0.40
1:C:322:ILE:HD13	1:C:338:TYR:CZ	2.57	0.40
1:D:214:ASP:C	1:D:214:ASP:OD2	2.60	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%)	13	27
1	B	338/368 (92%)	309 (91%)	24 (7%)	5 (2%)	10	21
1	C	331/368 (90%)	304 (92%)	25 (8%)	2 (1%)	25	47
1	D	336/368 (91%)	314 (94%)	22 (6%)	0	100	100
All	All	1343/1472 (91%)	1241 (92%)	91 (7%)	11 (1%)	19	39

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 [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	302/324 (93%)	294 (97%)	8 (3%)	46	72
1	B	302/324 (93%)	293 (97%)	9 (3%)	41	67
1	C	300/324 (93%)	292 (97%)	8 (3%)	44	71
1	D	301/324 (93%)	294 (98%)	7 (2%)	50	75
All	All	1205/1296 (93%)	1173 (97%)	32 (3%)	44	71

All (32) 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	400	ASP
1	A	418	PRO
1	A	480	LYS
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	400	ASP
1	B	481	LYS
1	C	167	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	400	ASP
1	D	167	LYS
1	D	226	ARG
1	D	278	THR
1	D	358	GLU
1	D	400	ASP
1	D	414	GLU
1	D	441	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	151	ASN
1	A	198	ASN
1	A	201	GLN
1	A	211	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	144	ASN
1	B	151	ASN
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	B	475	GLN
1	C	151	ASN
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	D	144	ASN
1	D	151	ASN
1	D	198	ASN
1	D	211	ASN
1	D	213	HIS
1	D	232	ASN
1	D	251	ASN
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 [i](#)

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	A	321	1	15,16,17	1.08	0	19,22,24	0.61	0
1	PTR	B	321	1	15,16,17	1.02	0	19,22,24	0.64	0
1	PTR	C	321	1	15,16,17	1.23	1 (6%)	19,22,24	0.61	0
1	PTR	D	321	1	15,16,17	1.04	0	19,22,24	0.67	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	A	321	1	-	0/10/11/13	0/1/1/1
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	C	321	1	-	2/10/11/13	0/1/1/1
1	PTR	D	321	1	-	0/10/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	321	PTR	P-OH	2.39	1.62	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (3) 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
1	B	321	PTR	CZ-OH-P-O2P

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 carbohydrates 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	A	1	-	18,18,18	2.89	12 (66%)	21,26,26	2.00	4 (19%)
2	HRM	B	1	-	18,18,18	2.74	7 (38%)	21,26,26	1.88	4 (19%)
2	HRM	C	1	-	18,18,18	2.94	7 (38%)	21,26,26	2.00	4 (19%)
2	HRM	D	1	-	18,18,18	2.73	9 (50%)	21,26,26	2.01	5 (23%)

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	A	1	-	-	0/2/2/2	0/3/3/3
2	HRM	B	1	-	-	0/2/2/2	0/3/3/3
2	HRM	C	1	-	-	0/2/2/2	0/3/3/3
2	HRM	D	1	-	-	0/2/2/2	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	HRM	CAL-NAH	7.98	1.39	1.32
2	B	1	HRM	CAL-NAH	7.50	1.38	1.32
2	A	1	HRM	CAL-NAH	7.13	1.38	1.32
2	D	1	HRM	CAL-NAH	5.45	1.37	1.32
2	C	1	HRM	CAG-CAK	5.00	1.46	1.37
2	D	1	HRM	CAD-CAK	4.37	1.47	1.38
2	D	1	HRM	CAG-CAK	4.21	1.44	1.37
2	B	1	HRM	CAG-CAK	3.96	1.44	1.37
2	A	1	HRM	CAB-CAL	3.69	1.53	1.50
2	C	1	HRM	CAE-CAC	3.66	1.41	1.36
2	D	1	HRM	CAF-CAD	3.63	1.44	1.36
2	D	1	HRM	CAE-CAC	3.60	1.41	1.36
2	B	1	HRM	CAE-CAC	3.58	1.41	1.36
2	A	1	HRM	CAF-CAD	3.53	1.44	1.36
2	C	1	HRM	CAF-CAD	3.34	1.43	1.36
2	B	1	HRM	CAD-CAK	3.27	1.45	1.38
2	D	1	HRM	CAB-CAL	3.14	1.52	1.50
2	A	1	HRM	CAE-CAC	3.06	1.40	1.36
2	A	1	HRM	CAG-CAK	3.03	1.42	1.37
2	A	1	HRM	CAG-CAM	-3.00	1.37	1.41
2	D	1	HRM	CAF-CAN	2.94	1.47	1.41
2	B	1	HRM	CAF-CAD	2.80	1.42	1.36
2	B	1	HRM	CAN-CAO	-2.78	1.37	1.45
2	A	1	HRM	CAN-CAO	-2.72	1.37	1.45
2	C	1	HRM	CAN-CAO	-2.65	1.38	1.45
2	C	1	HRM	CAF-CAN	2.63	1.46	1.41
2	C	1	HRM	CAD-CAK	2.61	1.43	1.38
2	A	1	HRM	CAL-CAP	-2.58	1.39	1.43
2	A	1	HRM	CAD-CAK	2.57	1.43	1.38
2	A	1	HRM	CAM-NAI	-2.43	1.31	1.38
2	B	1	HRM	CAC-NAH	2.41	1.39	1.34
2	A	1	HRM	OAJ-CAA	2.22	1.49	1.42
2	D	1	HRM	CAN-CAO	-2.18	1.39	1.45
2	A	1	HRM	CAF-CAN	2.18	1.45	1.41
2	D	1	HRM	CAC-NAH	2.07	1.39	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HRM	CAE-CAC-NAH	-4.85	119.03	123.81
2	C	1	HRM	CAE-CAC-NAH	-4.72	119.16	123.81
2	C	1	HRM	CAC-NAH-CAL	4.57	123.88	118.33
2	D	1	HRM	CAC-NAH-CAL	4.54	123.83	118.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HRM	CAC-NAH-CAL	4.34	123.59	118.33
2	B	1	HRM	CAE-CAC-NAH	-4.32	119.55	123.81
2	B	1	HRM	CAC-NAH-CAL	4.15	123.36	118.33
2	D	1	HRM	CAE-CAC-NAH	-4.10	119.77	123.81
2	D	1	HRM	CAF-CAN-CAM	3.83	123.25	118.17
2	C	1	HRM	CAF-CAN-CAM	3.81	123.22	118.17
2	B	1	HRM	CAF-CAN-CAM	3.81	123.22	118.17
2	A	1	HRM	CAF-CAN-CAM	3.62	122.97	118.17
2	A	1	HRM	CAD-CAF-CAN	-3.03	117.27	121.63
2	D	1	HRM	CAD-CAF-CAN	-2.56	117.94	121.63
2	B	1	HRM	CAD-CAF-CAN	-2.09	118.62	121.63
2	C	1	HRM	CAF-CAD-CAK	-2.03	117.44	120.17
2	D	1	HRM	CAF-CAD-CAK	-2.00	117.48	120.17

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	A	1	HRM	1	0
2	B	1	HRM	1	0
2	C	1	HRM	1	0
2	D	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	342/368 (92%)	-0.15	7 (2%) 65 60	13, 30, 59, 72	2 (0%)
1	B	342/368 (92%)	0.27	23 (6%) 17 13	15, 46, 83, 104	2 (0%)
1	C	337/368 (91%)	0.69	49 (14%) 2 1	21, 60, 97, 118	2 (0%)
1	D	340/368 (92%)	0.10	11 (3%) 47 40	19, 42, 67, 86	2 (0%)
All	All	1361/1472 (92%)	0.23	90 (6%) 18 13	13, 44, 86, 118	8 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	GLY	10.0
1	B	214	ASP	6.8
1	B	408	THR	6.5
1	C	413	ARG	5.9
1	B	215	THR	5.6
1	C	397	LYS	5.3
1	C	399	PRO	5.3
1	B	401	GLY	5.2
1	D	214	ASP	5.0
1	C	135	VAL	4.9
1	B	398	LEU	4.7
1	D	401	GLY	4.6
1	B	480	LYS	4.6
1	D	413	ARG	4.5
1	B	481	LYS	4.5
1	D	300	ARG	4.4
1	D	399	PRO	4.2
1	B	400	ASP	4.1
1	B	402	THR	4.1
1	C	433	GLY	3.9
1	C	402	THR	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	399	PRO	3.7
1	C	442	SER	3.6
1	A	214	ASP	3.6
1	D	135	VAL	3.6
1	C	481	LYS	3.5
1	B	407	LYS	3.5
1	B	216	GLU	3.4
1	C	398	LEU	3.4
1	B	133	ARG	3.4
1	A	481	LYS	3.3
1	C	400	ASP	3.3
1	C	253	ASN	3.3
1	A	135	VAL	3.2
1	A	215	THR	3.2
1	C	450	LEU	3.1
1	B	218	LYS	3.1
1	C	431	THR	3.0
1	C	432	GLY	3.0
1	C	446	VAL	3.0
1	C	382	ALA	2.9
1	D	398	LEU	2.9
1	C	386	ASP	2.9
1	C	417	PRO	2.9
1	C	299	LYS	2.9
1	D	136	TYR	2.8
1	C	300	ARG	2.8
1	B	179	ARG	2.7
1	B	415	TYR	2.6
1	C	477	SER	2.6
1	C	396	GLU	2.6
1	C	448	ASP	2.6
1	D	299	LYS	2.6
1	C	430	GLU	2.5
1	B	157	ASP	2.5
1	C	160	GLU	2.5
1	C	358	GLU	2.5
1	C	143	ASP	2.5
1	C	403	TRP	2.4
1	C	466	THR	2.4
1	A	134	LYS	2.4
1	C	392	ARG	2.4
1	C	472	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	415	TYR	2.4
1	C	444	HIS	2.3
1	A	216	GLU	2.3
1	C	475	GLN	2.3
1	C	383	HIS	2.3
1	C	214	ASP	2.3
1	C	414	GLU	2.3
1	B	299	LYS	2.2
1	C	436	GLY	2.2
1	D	253	ASN	2.2
1	C	480	LYS	2.2
1	B	254	PHE	2.2
1	C	134	LYS	2.2
1	B	300	ARG	2.2
1	C	381	PRO	2.2
1	A	408	THR	2.1
1	C	251	ASN	2.1
1	C	260	ASN	2.1
1	C	297	ASN	2.1
1	B	154	LYS	2.1
1	C	378	GLY	2.1
1	C	471	TYR	2.1
1	B	217	MET	2.1
1	D	400	ASP	2.1
1	C	286	CYS	2.0
1	C	405	LEU	2.0
1	B	459	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	PTR	C	321	16/17	0.93	0.13	31,42,44,46	0
1	PTR	B	321	16/17	0.97	0.12	38,45,46,50	0
1	PTR	D	321	16/17	0.98	0.12	26,28,31,33	0
1	PTR	A	321	16/17	0.99	0.12	16,22,29,36	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	HRM	B	1	16/16	0.97	0.14	15,20,26,30	0
2	HRM	C	1	16/16	0.97	0.13	27,33,40,42	0
2	HRM	D	1	16/16	0.97	0.13	24,31,34,35	0
2	HRM	A	1	16/16	0.99	0.15	5,11,16,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.