



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 11:16 pm BST

PDB ID : 3ANQ  
Title : human DYRK1A/inhibitor 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](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

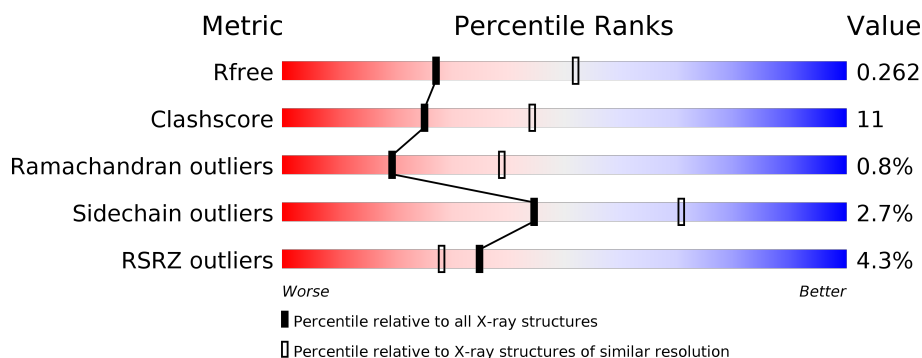
# 1 Overall quality at a glance

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	<div> <div> <div></div> <div>76%</div> <div>16%</div> <div>• 7%</div> </div> </div>
1	B	368	<div> <div>4%</div> <div>73%</div> <div>19%</div> <div>• 7%</div> </div>
1	C	368	<div> <div>7%</div> <div>73%</div> <div>19%</div> <div>• 7%</div> </div>
1	D	368	<div> <div>4%</div> <div>72%</div> <div>18%</div> <div>• 9%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11204 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.

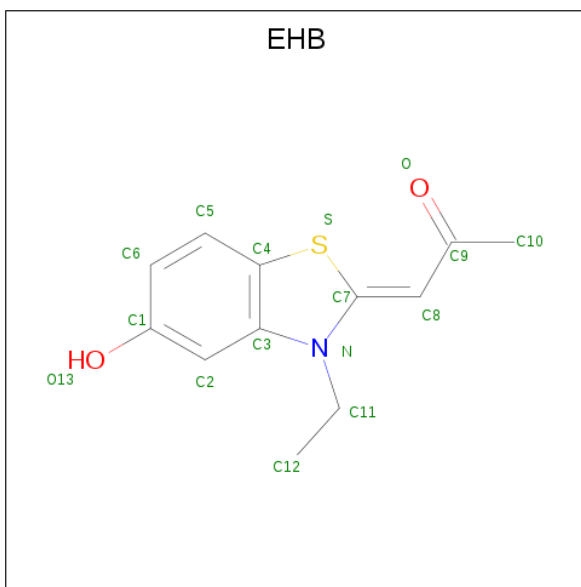
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	0	0	0
			2801	1804	479	500	1	17			
1	B	344	Total	C	N	O	P	S	0	0	0
			2802	1805	477	502	1	17			
1	C	341	Total	C	N	O	P	S	0	0	0
			2781	1792	473	498	1	17			
1	D	335	Total	C	N	O	P	S	0	0	0
			2736	1765	466	487	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 (1Z)-1-(3-ethyl-5-hydroxy-1,3-benzothiazol-2(3H)-ylidene)propan-2-one (three-letter code: EHB) (formula: C<sub>12</sub>H<sub>13</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	B	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	C	1	Total	C	N	O	S	0	0
			16	12	1	2	1		
2	D	1	Total	C	N	O	S	0	0
			16	12	1	2	1		

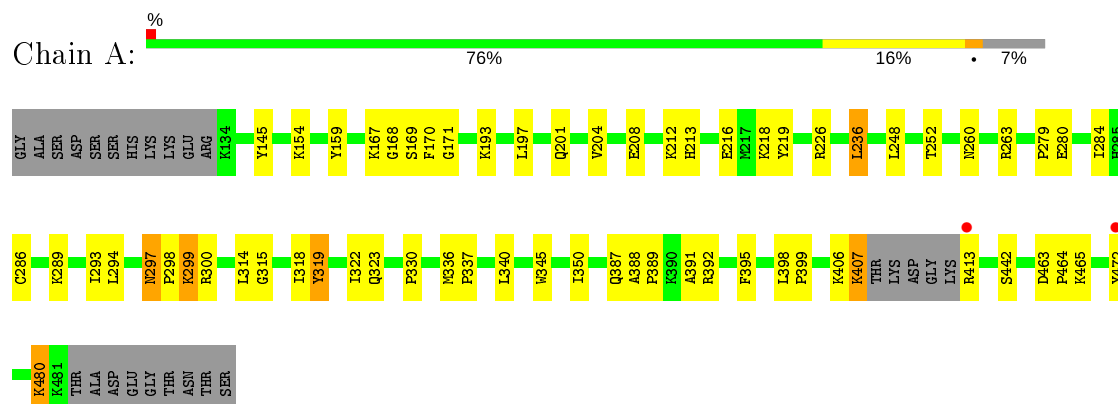
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	3	Total	O	0	0
			3	3		
3	C	4	Total	O	0	0
			4	4		
3	D	2	Total	O	0	0
			2	2		

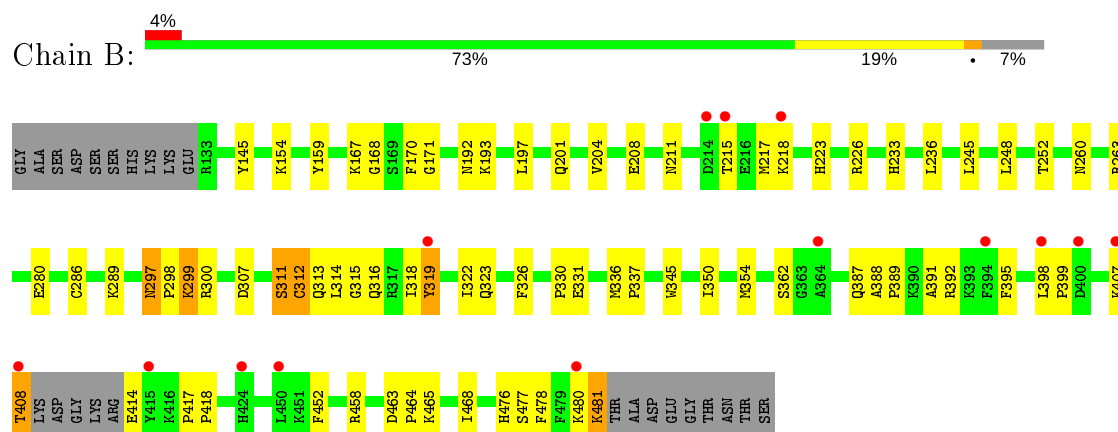
### 3 Residue-property plots

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.

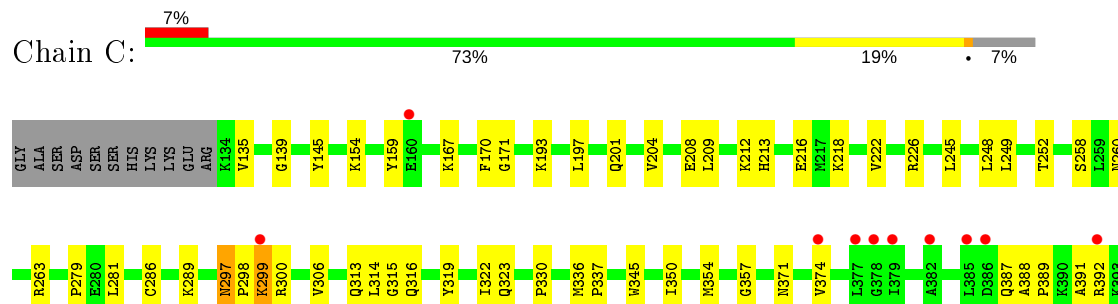
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

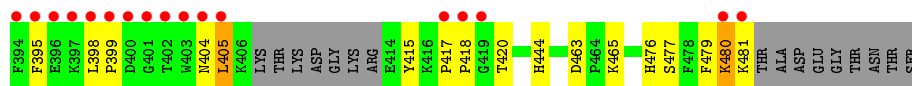


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

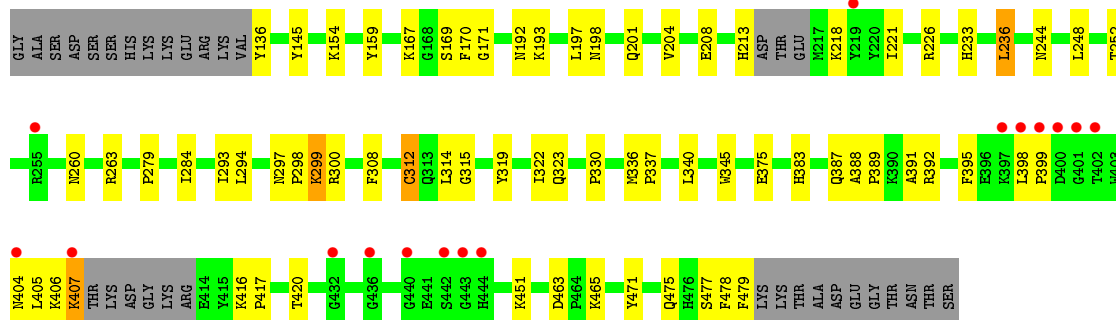


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





- 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, $\alpha$ , $\beta$ , $\gamma$	87.43Å 87.75Å 228.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.94 – 2.60 41.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (41.94-2.60) 97.2 (41.94-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.27 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.236 , 0.270 0.226 , 0.262	Depositor DCC
$R_{free}$ test set	2656 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 58.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11204	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EHB, 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	0.58	0/2849	0.69	0/3840
1	B	0.47	0/2850	0.64	0/3843
1	C	0.48	0/2829	0.64	0/3815
1	D	0.50	0/2783	0.65	0/3751
All	All	0.51	0/11311	0.66	0/15249

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	D	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	D	136	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	61	0
1	B	2802	0	2797	70	0
1	C	2781	0	2774	58	0
1	D	2736	0	2732	56	0
2	A	16	0	13	2	0
2	B	16	0	12	4	0
2	C	16	0	13	2	0
2	D	16	0	12	3	0
3	A	11	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
All	All	11204	0	11153	239	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 11.

All (239) 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:297:ASN:HD22	1:A:298:PRO:HD2	1.14	1.11
1:D:297:ASN:HD22	1:D:298:PRO:HD2	1.18	1.08
1:C:297:ASN:HD22	1:C:298:PRO:HD2	1.19	1.07
1:B:297:ASN:HD22	1:B:298:PRO:HD2	1.19	1.04
1:A:299:LYS:HZ3	1:A:299:LYS:HA	1.31	0.96
1:B:215:THR:HG22	1:B:217:MET:H	1.29	0.94
1:A:297:ASN:HD22	1:A:298:PRO:CD	1.82	0.92
1:C:297:ASN:HD22	1:C:298:PRO:CD	1.86	0.89
1:B:297:ASN:HD22	1:B:298:PRO:CD	1.85	0.89
1:A:299:LYS:NZ	1:A:299:LYS:HA	1.86	0.88
1:D:297:ASN:HD22	1:D:298:PRO:CD	1.87	0.87
1:B:299:LYS:NZ	1:B:299:LYS:HA	1.90	0.87
1:C:299:LYS:HA	1:C:299:LYS:NZ	1.90	0.84
1:D:299:LYS:HA	1:D:299:LYS:NZ	1.92	0.83
1:B:299:LYS:HA	1:B:299:LYS:HZ3	1.41	0.82
1:C:299:LYS:HZ3	1:C:299:LYS:HA	1.43	0.82
1:D:299:LYS:HA	1:D:299:LYS:HZ3	1.39	0.82
1:B:407:LYS:HG2	1:B:408:THR:H	1.43	0.82
1:A:407:LYS:NZ	1:A:407:LYS:HB3	1.94	0.81
1:A:407:LYS:HZ2	1:A:407:LYS:HB3	1.45	0.79
1:B:481:LYS:HE2	1:B:481:LYS:N	1.99	0.78
1:D:406:LYS:C	1:D:407:LYS:HD3	2.03	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:ND2	1:A:298:PRO:HD2	1.96	0.78
1:B:297:ASN:ND2	1:B:298:PRO:HD2	2.00	0.75
1:A:213:HIS:O	1:A:218:LYS:HD3	1.88	0.73
1:B:481:LYS:CE	1:B:481:LYS:H	2.02	0.73
1:D:297:ASN:ND2	1:D:298:PRO:HD2	2.00	0.72
1:B:314:LEU:O	1:C:315:GLY:HA3	1.89	0.72
1:A:406:LYS:O	1:A:407:LYS:HB3	1.90	0.71
1:A:201:GLN:HE22	1:B:318:ILE:CG2	2.04	0.70
1:C:477:SER:HA	1:C:480:LYS:HB2	1.73	0.70
1:C:297:ASN:ND2	1:C:298:PRO:HD2	2.00	0.69
1:D:375:GLU:OE2	1:D:416:LYS:HG3	1.92	0.68
1:B:481:LYS:HE2	1:B:481:LYS:H	1.58	0.68
1:D:387:GLN:O	1:D:389:PRO:HD3	1.94	0.68
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.76	0.68
1:C:479:PHE:O	1:C:481:LYS:N	2.27	0.68
1:D:407:LYS:N	1:D:407:LYS:HD3	2.07	0.68
1:B:337:PRO:HG3	1:C:279:PRO:HG3	1.76	0.67
1:A:279:PRO:HG3	1:D:337:PRO:HG3	1.75	0.67
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.78	0.65
1:C:417:PRO:HB2	1:C:420:THR:HG21	1.79	0.64
1:C:371:ASN:HB3	1:C:415:TYR:CD2	2.32	0.64
1:C:387:GLN:O	1:C:389:PRO:HD3	1.98	0.64
1:A:284:ILE:HG12	1:A:340:LEU:HD12	1.80	0.64
2:C:1:EHB:H8	2:C:1:EHB:C12	2.28	0.64
1:A:297:ASN:ND2	1:A:298:PRO:CD	2.59	0.62
1:A:322:ILE:O	1:A:323:GLN:HB2	1.98	0.62
2:D:1:EHB:H8	2:D:1:EHB:C12	2.30	0.61
2:B:1:EHB:H8	2:B:1:EHB:C12	2.31	0.61
1:B:387:GLN:O	1:B:389:PRO:HD3	2.00	0.61
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.82	0.61
1:B:215:THR:HG22	1:B:217:MET:N	2.11	0.61
1:B:480:LYS:HA	1:B:481:LYS:NZ	2.15	0.61
1:B:407:LYS:HG2	1:B:408:THR:N	2.13	0.60
1:D:388:ALA:HB3	1:D:391:ALA:HB2	1.83	0.60
1:A:169:SER:HB3	1:B:145:TYR:OH	2.02	0.59
1:B:398:LEU:HB3	1:B:399:PRO:HD2	1.83	0.59
1:C:398:LEU:HB3	1:C:399:PRO:HD2	1.84	0.59
1:B:314:LEU:HG	1:B:315:GLY:N	2.17	0.59
1:B:481:LYS:CD	1:B:481:LYS:H	2.16	0.59
1:C:374:VAL:HG11	1:C:405:LEU:HD21	1.84	0.59
1:D:398:LEU:HB3	1:D:399:PRO:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:O	1:B:312:CYS:HB3	2.04	0.58
1:A:299:LYS:NZ	1:A:299:LYS:CA	2.66	0.57
1:B:211:ASN:OD1	1:B:223:HIS:HD2	1.88	0.56
1:C:281:LEU:O	1:C:313:GLN:NE2	2.33	0.56
1:A:300:ARG:HG3	1:A:300:ARG:HH11	1.71	0.56
1:C:398:LEU:HG	1:C:404:ASN:HD22	1.71	0.56
1:A:145:TYR:CE1	1:A:193:LYS:HD3	2.41	0.56
1:C:297:ASN:ND2	1:C:298:PRO:CD	2.63	0.55
1:D:300:ARG:HG3	1:D:300:ARG:HH11	1.72	0.55
1:B:307:ASP:HB2	2:B:1:EHB:H10B	1.89	0.55
1:C:204:VAL:O	1:C:208:GLU:HG3	2.07	0.55
1:C:222:VAL:HB	1:C:306:VAL:HG12	1.89	0.55
1:C:300:ARG:HG3	1:C:300:ARG:HH11	1.71	0.55
1:C:322:ILE:O	1:C:323:GLN:HB2	2.06	0.54
1:A:398:LEU:HB3	1:A:399:PRO:HD2	1.88	0.54
1:D:336:MET:HB3	1:D:337:PRO:CD	2.38	0.54
1:C:417:PRO:HB2	1:C:420:THR:CG2	2.37	0.54
1:D:204:VAL:O	1:D:208:GLU:HG3	2.07	0.54
1:C:404:ASN:O	1:C:405:LEU:O	2.25	0.54
1:D:145:TYR:CE1	1:D:193:LYS:HD3	2.42	0.54
1:B:260:ASN:HA	1:B:263:ARG:NH1	2.24	0.53
1:B:297:ASN:ND2	1:B:298:PRO:CD	2.62	0.53
1:C:299:LYS:HZ2	1:C:299:LYS:HA	1.73	0.53
1:A:387:GLN:O	1:A:389:PRO:HD3	2.08	0.53
1:A:314:LEU:O	1:D:315:GLY:HA2	2.09	0.53
1:B:452:PHE:HB2	1:B:478:PHE:CE1	2.44	0.53
1:A:318:ILE:HG13	1:A:319:TYR:CE1	2.44	0.53
1:C:336:MET:HB3	1:C:337:PRO:CD	2.38	0.53
1:A:204:VAL:O	1:A:208:GLU:HG3	2.09	0.52
1:C:371:ASN:HB3	1:C:415:TYR:HD2	1.71	0.52
1:B:263:ARG:HG3	1:B:478:PHE:CE2	2.44	0.52
1:B:260:ASN:HA	1:B:263:ARG:HH12	1.73	0.52
1:A:480:LYS:HB3	1:A:480:LYS:HZ2	1.73	0.52
1:B:300:ARG:HG3	1:B:300:ARG:HH11	1.75	0.52
1:C:145:TYR:CE1	1:C:193:LYS:HD3	2.44	0.52
1:B:299:LYS:NZ	1:B:299:LYS:CA	2.70	0.52
1:D:297:ASN:ND2	1:D:298:PRO:CD	2.64	0.52
1:A:472:TYR:OH	1:D:383:HIS:HB2	2.10	0.52
1:D:260:ASN:HA	1:D:263:ARG:HH12	1.73	0.52
1:D:451:LYS:HD3	1:D:477:SER:OG	2.10	0.52
1:D:260:ASN:HA	1:D:263:ARG:NH1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:O	1:A:407:LYS:CB	2.55	0.51
1:C:209:LEU:O	1:C:212:LYS:HB3	2.10	0.51
1:D:398:LEU:HD11	1:D:404:ASN:ND2	2.25	0.51
1:A:336:MET:HB3	1:A:337:PRO:CD	2.40	0.51
1:C:145:TYR:OH	1:D:169:SER:HB3	2.10	0.50
1:B:477:SER:HA	1:B:480:LYS:HG3	1.94	0.50
1:D:471:TYR:CZ	1:D:475:GLN:NE2	2.80	0.50
1:B:336:MET:HB3	1:B:337:PRO:CD	2.41	0.50
1:A:407:LYS:HG2	1:A:407:LYS:O	2.11	0.50
1:B:145:TYR:CE1	1:B:193:LYS:HD3	2.47	0.50
1:B:204:VAL:O	1:B:208:GLU:HG3	2.11	0.50
1:D:314:LEU:HD12	1:D:315:GLY:H	1.76	0.50
1:D:213:HIS:C	1:D:218:LYS:NZ	2.65	0.49
1:A:318:ILE:HG13	1:A:319:TYR:CD1	2.47	0.49
2:C:1:EHB:H8	2:C:1:EHB:H12B	1.94	0.49
1:A:284:ILE:CG1	1:A:340:LEU:HD12	2.41	0.49
1:C:260:ASN:HA	1:C:263:ARG:NH1	2.27	0.49
1:C:213:HIS:O	1:C:218:LYS:HD3	2.13	0.49
1:C:197:LEU:O	1:C:201:GLN:HG3	2.13	0.48
1:B:299:LYS:HA	1:B:299:LYS:HZ2	1.75	0.48
1:C:260:ASN:HA	1:C:263:ARG:HH12	1.78	0.48
2:B:1:EHB:S	2:B:1:EHB:O	2.71	0.48
1:B:331:GLU:OE2	1:B:464:PRO:HB3	2.13	0.48
1:B:480:LYS:HA	1:B:481:LYS:HZ3	1.79	0.48
1:A:260:ASN:HA	1:A:263:ARG:NH1	2.29	0.48
1:D:314:LEU:HD12	1:D:315:GLY:N	2.29	0.48
1:D:417:PRO:HB2	1:D:420:THR:HG21	1.96	0.48
1:D:197:LEU:O	1:D:201:GLN:HG3	2.14	0.47
1:A:154:LYS:HA	1:A:159:TYR:O	2.14	0.47
1:A:407:LYS:NZ	1:A:407:LYS:CB	2.71	0.47
2:A:1:EHB:O	2:A:1:EHB:S	2.72	0.47
1:C:371:ASN:HB3	1:C:415:TYR:CE2	2.50	0.47
1:B:197:LEU:O	1:B:201:GLN:HG3	2.15	0.47
1:C:398:LEU:CD1	1:C:404:ASN:ND2	2.78	0.47
1:D:322:ILE:O	1:D:323:GLN:HB2	2.13	0.47
1:A:260:ASN:HA	1:A:263:ARG:HH12	1.80	0.47
1:C:330:PRO:HD3	1:C:345:TRP:CE2	2.50	0.46
1:A:472:TYR:CZ	1:D:383:HIS:HB2	2.50	0.46
1:A:463:ASP:OD1	1:A:465:LYS:HB2	2.15	0.46
1:B:417:PRO:HA	1:B:418:PRO:HD3	1.66	0.46
1:D:145:TYR:CD1	1:D:193:LYS:HD3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:EHB:H8	2:A:1:EHB:C12	2.45	0.46
1:B:477:SER:HA	1:B:480:LYS:CG	2.46	0.46
1:C:299:LYS:NZ	1:C:299:LYS:CA	2.70	0.46
1:A:315:GLY:HA2	1:D:314:LEU:O	2.16	0.46
1:B:248:LEU:O	1:B:252:THR:HG23	2.16	0.46
1:C:371:ASN:CB	1:C:415:TYR:CE2	2.97	0.46
1:D:330:PRO:HD3	1:D:345:TRP:CE2	2.51	0.46
1:B:476:HIS:O	1:B:480:LYS:HG3	2.16	0.46
1:B:463:ASP:OD1	1:B:465:LYS:HB2	2.15	0.46
1:C:463:ASP:OD1	1:C:465:LYS:HB2	2.15	0.46
1:B:311:SER:O	1:B:312:CYS:CB	2.63	0.46
1:C:135:VAL:HG13	1:C:139:GLY:N	2.31	0.46
1:C:154:LYS:HA	1:C:159:TYR:O	2.16	0.45
1:A:413:ARG:O	1:A:413:ARG:HG2	2.16	0.45
1:A:248:LEU:O	1:A:252:THR:HG23	2.15	0.45
1:D:392:ARG:HA	1:D:395:PHE:O	2.17	0.45
1:D:463:ASP:OD1	1:D:465:LYS:HB2	2.15	0.45
1:A:216:GLU:OE2	1:A:216:GLU:N	2.50	0.45
1:B:477:SER:HA	1:B:480:LYS:HD3	1.98	0.45
1:C:216:GLU:O	1:C:216:GLU:HG2	2.17	0.45
1:D:213:HIS:C	1:D:218:LYS:HD3	2.36	0.45
1:A:197:LEU:HD23	1:B:319:TYR:CD1	2.51	0.45
1:C:289:LYS:HA	1:C:350:ILE:HD11	1.98	0.45
1:A:145:TYR:CD1	1:A:193:LYS:HD3	2.51	0.45
1:A:280:GLU:N	1:A:280:GLU:OE1	2.40	0.45
1:B:245:LEU:HB3	1:B:354:MET:HE1	1.99	0.44
1:D:248:LEU:O	1:D:252:THR:HG23	2.17	0.44
1:B:314:LEU:CG	1:B:315:GLY:N	2.80	0.44
1:B:452:PHE:HB2	1:B:478:PHE:HE1	1.83	0.44
1:C:248:LEU:O	1:C:252:THR:HG23	2.17	0.44
1:B:322:ILE:O	1:B:323:GLN:HB2	2.17	0.44
1:B:477:SER:HA	1:B:480:LYS:CD	2.47	0.44
1:C:258:SER:HB2	1:C:444:HIS:CE1	2.52	0.44
1:B:326:PHE:CD1	1:B:362:SER:HA	2.53	0.44
1:C:415:TYR:N	1:C:415:TYR:HD1	2.16	0.44
1:D:154:LYS:HA	1:D:159:TYR:O	2.16	0.44
1:C:415:TYR:N	1:C:415:TYR:CD1	2.86	0.43
1:A:197:LEU:HD23	1:B:319:TYR:HD1	1.83	0.43
1:B:168:GLY:HA3	1:B:170:PHE:CE2	2.53	0.43
1:D:336:MET:HB3	1:D:337:PRO:HD2	1.99	0.43
1:C:170:PHE:CD1	1:C:171:GLY:N	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:O	1:A:201:GLN:HG3	2.17	0.43
1:A:216:GLU:HG3	1:A:219:TYR:HE2	1.83	0.43
1:D:417:PRO:HB2	1:D:420:THR:CG2	2.48	0.43
1:B:215:THR:O	1:B:218:LYS:HG2	2.18	0.43
1:D:244:ASN:HA	1:D:294:LEU:HA	2.00	0.43
1:D:293:ILE:C	1:D:294:LEU:HD12	2.39	0.43
1:D:284:ILE:HG12	1:D:340:LEU:HD12	2.00	0.43
1:B:280:GLU:OE1	1:B:280:GLU:N	2.43	0.43
1:B:154:LYS:HA	1:B:159:TYR:O	2.19	0.43
1:D:398:LEU:HD11	1:D:404:ASN:HD22	1.83	0.43
1:B:297:ASN:HD22	1:B:298:PRO:N	2.16	0.43
1:A:337:PRO:HG3	1:D:279:PRO:HG3	2.00	0.43
1:D:221:ILE:HG23	1:D:308:PHE:CE2	2.54	0.42
1:A:392:ARG:HA	1:A:395:PHE:O	2.19	0.42
1:B:330:PRO:HD3	1:B:345:TRP:CE2	2.53	0.42
1:C:392:ARG:HA	1:C:395:PHE:O	2.20	0.42
1:D:170:PHE:CD1	1:D:171:GLY:N	2.87	0.42
1:B:170:PHE:CD1	1:B:171:GLY:N	2.88	0.42
1:B:458:ARG:O	1:B:468:ILE:HG22	2.19	0.42
1:A:293:ILE:C	1:A:294:LEU:HD12	2.40	0.42
2:D:1:EHB:H8	2:D:1:EHB:H12A	2.01	0.42
1:C:145:TYR:CD1	1:C:193:LYS:HD3	2.54	0.42
2:B:1:EHB:H8	2:B:1:EHB:H12B	1.99	0.42
1:D:477:SER:O	1:D:479:PHE:N	2.52	0.42
1:A:472:TYR:OH	1:D:383:HIS:CD2	2.73	0.42
1:A:297:ASN:HD22	1:A:298:PRO:N	2.17	0.42
1:C:371:ASN:CB	1:C:415:TYR:HE2	2.33	0.42
1:A:168:GLY:HA3	1:A:170:PHE:CE2	2.55	0.41
1:A:299:LYS:HZ2	1:A:299:LYS:HA	1.81	0.41
1:B:145:TYR:CD1	1:B:193:LYS:HD3	2.53	0.41
1:D:192:ASN:HB2	1:D:233:HIS:CE1	2.55	0.41
1:A:170:PHE:CD1	1:A:171:GLY:N	2.89	0.41
1:C:245:LEU:HB3	1:C:354:MET:HE1	2.02	0.41
1:C:417:PRO:O	1:C:418:PRO:C	2.59	0.41
1:D:330:PRO:HD3	1:D:345:TRP:CD2	2.55	0.41
2:D:1:EHB:H8	2:D:1:EHB:H12B	2.01	0.41
1:A:236:LEU:N	1:A:236:LEU:HD23	2.36	0.41
1:A:330:PRO:HD3	1:A:345:TRP:CE2	2.56	0.41
1:D:312:CYS:HB3	1:D:319:TYR:HE2	1.86	0.41
1:A:201:GLN:HE22	1:B:318:ILE:HG22	1.82	0.41
1:A:336:MET:HB3	1:A:337:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:HA	1:B:350:ILE:HD11	2.02	0.41
1:B:392:ARG:HA	1:B:395:PHE:O	2.20	0.41
1:A:289:LYS:HA	1:A:350:ILE:HD11	2.03	0.41
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.56	0.41
1:B:480:LYS:HB3	1:B:480:LYS:HE2	1.89	0.40
1:C:336:MET:HB3	1:C:337:PRO:HD2	2.02	0.40
1:A:463:ASP:HA	1:A:464:PRO:HD2	1.99	0.40
1:C:319:TYR:HE1	1:D:198:ASN:HD21	1.69	0.40
1:C:330:PRO:HD3	1:C:345:TRP:CD2	2.56	0.40
1:D:236:LEU:HD23	1:D:236:LEU:N	2.36	0.40
1:B:336:MET:HB3	1:B:337:PRO:HD2	2.04	0.40
1:C:249:LEU:HD22	1:C:357:GLY:HA2	2.03	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%)	318 (94%)	20 (6%)	0	100	100
1	B	339/368 (92%)	315 (93%)	20 (6%)	4 (1%)	13	27
1	C	336/368 (91%)	302 (90%)	29 (9%)	5 (2%)	10	21
1	D	328/368 (89%)	303 (92%)	23 (7%)	2 (1%)	25	47
All	All	1341/1472 (91%)	1238 (92%)	92 (7%)	11 (1%)	19	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	312	CYS
1	C	405	LEU
1	C	480	LYS

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Mol	Chain	Res	Type
1	B	311	SER
1	B	316	GLN
1	C	316	GLN
1	D	478	PHE
1	C	476	HIS
1	D	405	LEU
1	C	314	LEU
1	B	313	GLN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	301/324 (93%)	290 (96%)	11 (4%)	34	60
1	B	301/324 (93%)	291 (97%)	10 (3%)	38	64
1	C	299/324 (92%)	294 (98%)	5 (2%)	60	81
1	D	294/324 (91%)	288 (98%)	6 (2%)	55	78
All	All	1195/1296 (92%)	1163 (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	212	LYS
1	A	226	ARG
1	A	236	LEU
1	A	286	CYS
1	A	297	ASN
1	A	299	LYS
1	A	319	TYR
1	A	407	LYS
1	A	442	SER
1	A	480	LYS
1	B	167	LYS
1	B	226	ARG

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Mol	Chain	Res	Type
1	B	236	LEU
1	B	286	CYS
1	B	297	ASN
1	B	299	LYS
1	B	319	TYR
1	B	408	THR
1	B	414	GLU
1	B	481	LYS
1	C	167	LYS
1	C	226	ARG
1	C	286	CYS
1	C	297	ASN
1	C	299	LYS
1	D	167	LYS
1	D	226	ARG
1	D	236	LEU
1	D	299	LYS
1	D	312	CYS
1	D	407	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	ASN
1	A	201	GLN
1	A	211	ASN
1	A	223	HIS
1	A	232	ASN
1	A	297	ASN
1	A	320	GLN
1	A	387	GLN
1	A	404	ASN
1	A	425	ASN
1	B	198	ASN
1	B	213	HIS
1	B	223	HIS
1	B	232	ASN
1	B	297	ASN
1	B	404	ASN
1	B	425	ASN
1	C	198	ASN
1	C	211	ASN

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Mol	Chain	Res	Type
1	C	223	HIS
1	C	232	ASN
1	C	297	ASN
1	C	320	GLN
1	C	404	ASN
1	C	425	ASN
1	D	198	ASN
1	D	211	ASN
1	D	213	HIS
1	D	232	ASN
1	D	297	ASN
1	D	383	HIS
1	D	387	GLN
1	D	404	ASN
1	D	425	ASN
1	D	475	GLN

### 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	B	321	1	15,16,17	1.67	4 (26%)	19,22,24	0.72	0
1	PTR	A	321	1	15,16,17	1.29	3 (20%)	19,22,24	0.72	0
1	PTR	D	321	1	15,16,17	1.17	0	19,22,24	0.83	1 (5%)
1	PTR	C	321	1	15,16,17	1.14	1 (6%)	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	B	321	1	-	0/10/11/13	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	C	321	1	-	0/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	PTR	CE2-CD2	3.01	1.44	1.38
1	B	321	PTR	P-OH	2.72	1.63	1.59
1	A	321	PTR	CE2-CZ	2.41	1.43	1.38
1	A	321	PTR	CE2-CD2	2.28	1.42	1.38
1	B	321	PTR	CD2-CG	2.24	1.43	1.38
1	C	321	PTR	P-OH	2.12	1.62	1.59
1	A	321	PTR	CE1-CZ	2.03	1.42	1.38
1	B	321	PTR	CE1-CD1	2.00	1.42	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	PTR	O2P-P-O1P	2.06	118.74	110.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	EHB	D	1	-	14,17,17	9.87	2 (14%)	12,24,24	1.68	2 (16%)
2	EHB	C	1	-	14,17,17	9.60	1 (7%)	12,24,24	1.66	1 (8%)
2	EHB	B	1	-	14,17,17	8.98	2 (14%)	12,24,24	1.48	1 (8%)
2	EHB	A	1	-	14,17,17	8.57	1 (7%)	12,24,24	1.61	2 (16%)

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	EHB	D	1	-	-	2/4/6/6	0/2/2/2
2	EHB	C	1	-	-	2/4/6/6	0/2/2/2
2	EHB	B	1	-	-	2/4/6/6	0/2/2/2
2	EHB	A	1	-	-	2/4/6/6	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	EHB	C4-S	-36.72	1.45	1.74
2	C	1	EHB	C4-S	-35.78	1.46	1.74
2	B	1	EHB	C4-S	-33.42	1.48	1.74
2	A	1	EHB	C4-S	-31.95	1.49	1.74
2	D	1	EHB	C7-N	-2.13	1.34	1.38
2	B	1	EHB	C8-C9	-2.02	1.37	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	EHB	C12-C11-N	4.87	119.72	111.49
2	A	1	EHB	C12-C11-N	4.78	119.57	111.49
2	D	1	EHB	C12-C11-N	4.62	119.30	111.49
2	B	1	EHB	C12-C11-N	4.37	118.87	111.49
2	A	1	EHB	C5-C4-S	2.07	129.31	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	EHB	C2-C3-C4	-2.03	118.85	120.56

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	EHB	C12-C11-N-C3
2	D	1	EHB	C12-C11-N-C7
2	C	1	EHB	C12-C11-N-C3
2	C	1	EHB	C12-C11-N-C7
2	B	1	EHB	C12-C11-N-C3
2	B	1	EHB	C12-C11-N-C7
2	A	1	EHB	C12-C11-N-C3
2	A	1	EHB	C12-C11-N-C7

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	EHB	3	0
2	C	1	EHB	2	0
2	B	1	EHB	4	0
2	A	1	EHB	2	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%)	-0.31	2 (0%) 89 88	24, 40, 72, 91	2 (0%)
1	B	343/368 (93%)	0.21	14 (4%) 37 30	33, 67, 101, 121	2 (0%)
1	C	340/368 (92%)	0.21	27 (7%) 12 9	29, 66, 109, 133	2 (0%)
1	D	334/368 (90%)	0.19	16 (4%) 30 24	31, 62, 104, 119	2 (0%)
All	All	1359/1472 (92%)	0.07	59 (4%) 35 28	24, 60, 103, 133	8 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	401	GLY	7.0
1	D	440	GLY	6.0
1	C	399	PRO	5.6
1	C	402	THR	5.3
1	D	398	LEU	4.8
1	C	385	LEU	4.7
1	C	382	ALA	4.6
1	C	398	LEU	4.6
1	C	405	LEU	4.5
1	D	399	PRO	4.5
1	D	443	GLY	4.5
1	D	401	GLY	4.4
1	D	402	THR	4.4
1	C	400	ASP	4.4
1	B	398	LEU	3.8
1	C	396	GLU	3.7
1	D	436	GLY	3.6
1	C	404	ASN	3.6
1	C	397	LYS	3.5
1	C	395	PHE	3.4
1	B	480	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	432	GLY	3.3
1	D	442	SER	3.3
1	B	415	TYR	3.2
1	C	379	ILE	3.1
1	C	403	TRP	3.1
1	B	407	LYS	3.1
1	B	214	ASP	2.8
1	C	481	LYS	2.8
1	B	400	ASP	2.7
1	B	450	LEU	2.7
1	C	377	LEU	2.7
1	D	400	ASP	2.6
1	D	397	LYS	2.6
1	B	218	LYS	2.6
1	A	413	ARG	2.5
1	B	319	TYR	2.5
1	C	480	LYS	2.4
1	D	407	LYS	2.4
1	C	392	ARG	2.4
1	B	424	HIS	2.3
1	C	419	GLY	2.3
1	D	404	ASN	2.3
1	C	417	PRO	2.2
1	D	255	ARG	2.2
1	A	472	TYR	2.2
1	C	160	GLU	2.1
1	B	394	PHE	2.1
1	C	394	PHE	2.1
1	C	299	LYS	2.1
1	C	386	ASP	2.1
1	B	408	THR	2.1
1	C	374	VAL	2.1
1	C	418	PRO	2.1
1	D	219	TYR	2.1
1	B	364	ALA	2.1
1	B	215	THR	2.1
1	D	444	HIS	2.0
1	C	378	GLY	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	B	321	16/17	0.97	0.14	48,59,63,64	0
1	PTR	D	321	16/17	0.97	0.12	35,40,44,46	0
1	PTR	C	321	16/17	0.97	0.12	45,56,66,66	0
1	PTR	A	321	16/17	0.98	0.13	31,41,44,46	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	EHB	D	1	16/16	0.95	0.19	48,58,63,69	0
2	EHB	C	1	16/16	0.95	0.16	38,45,53,53	0
2	EHB	B	1	16/16	0.96	0.16	35,44,61,61	0
2	EHB	A	1	16/16	0.96	0.16	33,37,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.