



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:50 PM GMT

PDB ID : 2WPC  
Title : TRYPANOSOMA BRUCEI TRYPANOTHIONE REDUCTASE IN COM-  
PLEX WITH 3,4-DIHYDROQUINAZOLINEINHIBITOR (DDD00073357)  
Authors : Alphey, M.S.; Patterson, S.; Fairlamb, A.H.  
Deposited on : 2009-08-05  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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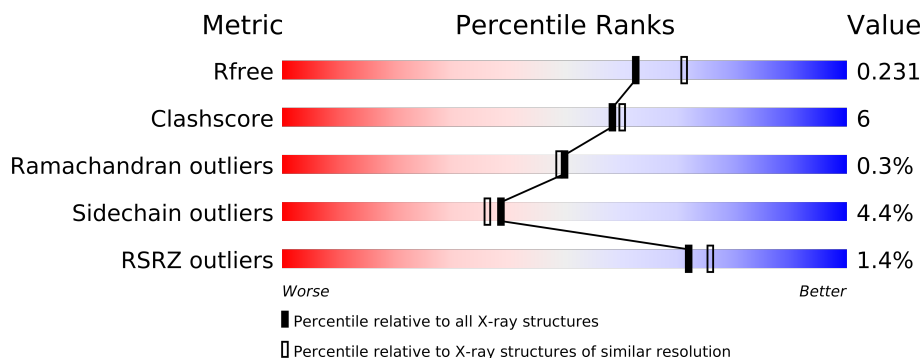
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	495	
1	B	495	
1	C	495	
1	D	495	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	WP7	A	1000	-	X
5	NA	B	2005	-	X
5	NA	D	1492	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16689 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

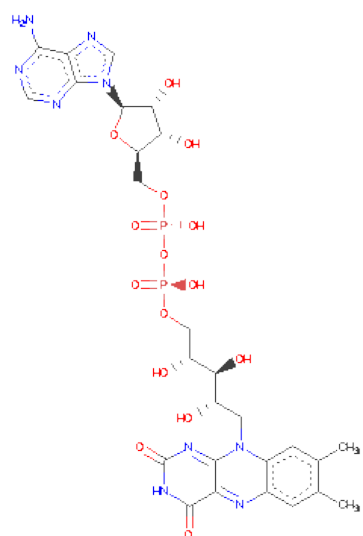
- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3715	2362	632	701	20			
1	B	487	Total	C	N	O	S	0	3	0
			3716	2365	634	698	19			
1	C	492	Total	C	N	O	S	0	1	0
			3740	2378	636	706	20			
1	D	490	Total	C	N	O	S	0	1	0
			3728	2371	633	704	20			

There are 12 discrepancies between the modelled and reference sequences:

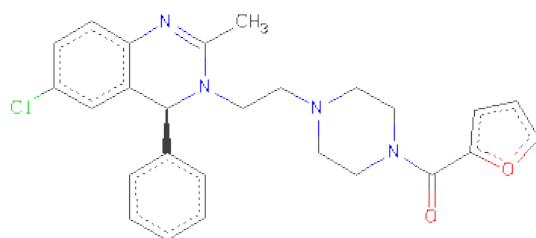
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q389T8
A	-1	SER	-	EXPRESSION TAG	UNP Q389T8
A	0	HIS	-	EXPRESSION TAG	UNP Q389T8
B	-2	GLY	-	EXPRESSION TAG	UNP Q389T8
B	-1	SER	-	EXPRESSION TAG	UNP Q389T8
B	0	HIS	-	EXPRESSION TAG	UNP Q389T8
C	-2	GLY	-	EXPRESSION TAG	UNP Q389T8
C	-1	SER	-	EXPRESSION TAG	UNP Q389T8
C	0	HIS	-	EXPRESSION TAG	UNP Q389T8
D	-2	GLY	-	EXPRESSION TAG	UNP Q389T8
D	-1	SER	-	EXPRESSION TAG	UNP Q389T8
D	0	HIS	-	EXPRESSION TAG	UNP Q389T8

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is (4S)-6-CHLORO-3-{2-[4-(FURAN-2-YLCARBONYL)PIPERAZIN-1-YL]ETHYL}-2-METHYL-4-PHENYL-3,4-DIHYDROQUINAZOLINE (three-letter code: WP7) (formula: C<sub>26</sub>H<sub>27</sub>ClN<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	
			33	26	1	4	2	
3	B	1	Total	C	Cl	N	O	
			33	26	1	4	2	
3	C	1	Total	C	Cl	N	O	
			33	26	1	4	2	
3	D	1	Total	C	Cl	N	O	
			33	26	1	4	2	

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Na		
			2	2	0	0
5	A	2	Total	Na		
			2	2	0	0
5	D	2	Total	Na		
			2	2	0	0
5	C	2	Total	Na		
			2	2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	364	Total	O		
			364	364	0	0
6	B	343	Total	O		
			343	343	0	0
6	C	350	Total	O		
			350	350	0	0

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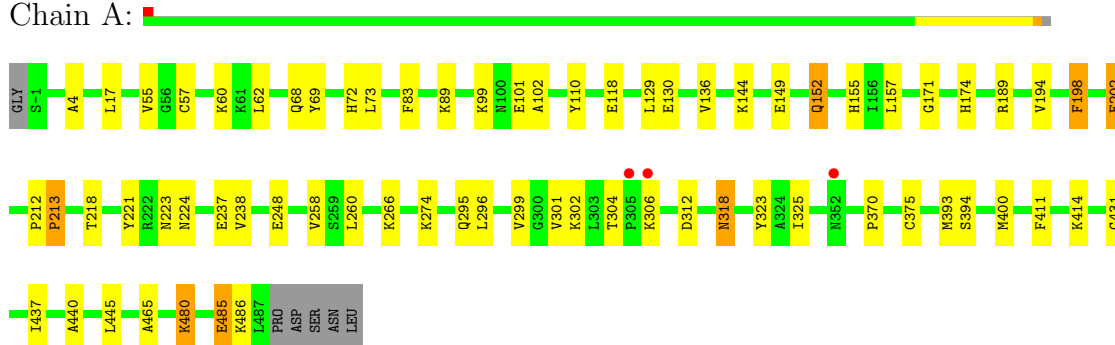
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	370	Total	O	0	0
			370	370		

### 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 errors 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.

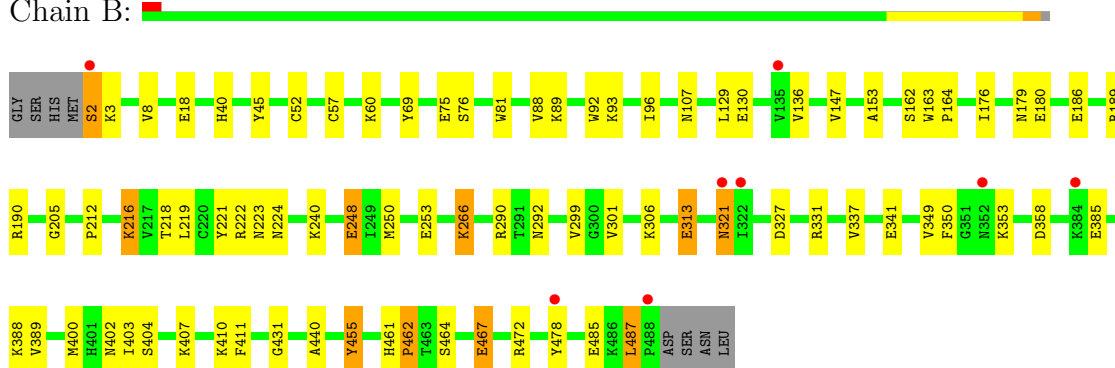
#### • Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



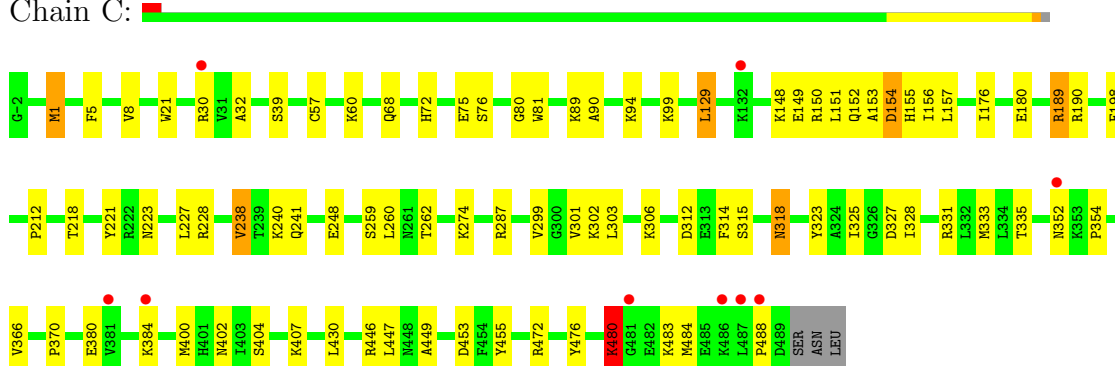
#### • Molecule 1: TRYPANOTHIONE REDUCTASE

Chain B:



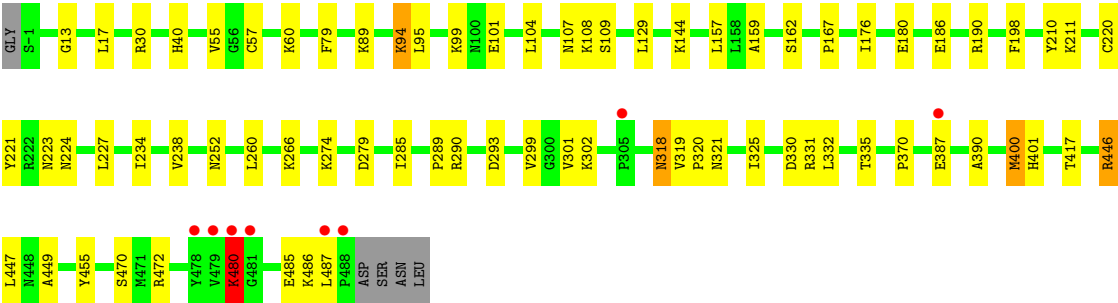
#### • Molecule 1: TRYPANOTHIONE REDUCTASE

Chain C:



● Molecule 1: TRYPANOTHIONE REDUCTASE

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.25Å 63.43Å 169.37Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	46.88 – 2.10 46.86 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.88-2.10) 94.2 (46.86-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.165 , 0.232 0.165 , 0.231	Depositor DCC
$R_{free}$ test set	5868 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 117358 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16689	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, WP7, FAD, CL

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	1.16	7/3793 (0.2%)	0.94	1/5144 (0.0%)
1	B	1.08	4/3803 (0.1%)	0.91	4/5158 (0.1%)
1	C	1.08	0/3822	0.90	4/5183 (0.1%)
1	D	1.14	6/3810 (0.2%)	0.92	2/5168 (0.0%)
All	All	1.12	17/15228 (0.1%)	0.92	11/20653 (0.1%)

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	B	0	1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	GLU	CG-CD	5.97	1.60	1.51
1	D	220	CYS	CB-SG	-5.80	1.72	1.81
1	A	110	TYR	CE1-CZ	5.78	1.46	1.38
1	A	102	ALA	CA-CB	5.76	1.64	1.52
1	D	198	PHE	CE1-CZ	5.75	1.48	1.37
1	B	205	GLY	N-CA	5.71	1.54	1.46
1	A	194	VAL	CB-CG2	5.47	1.64	1.52
1	B	69	TYR	CE2-CZ	5.32	1.45	1.38
1	D	109	SER	CB-OG	-5.30	1.35	1.42
1	D	162	SER	CB-OG	5.29	1.49	1.42
1	B	248	GLU	CD-OE1	5.27	1.31	1.25
1	B	455	TYR	CD1-CE1	5.27	1.47	1.39
1	D	159	ALA	CA-CB	5.15	1.63	1.52
1	A	202	GLU	CB-CG	5.10	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	PHE	CD1-CE1	5.04	1.49	1.39
1	A	149	GLU	CG-CD	5.03	1.59	1.51
1	D	79	PHE	CE2-CZ	5.02	1.46	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	LYS	CD-CE-NZ	-7.18	95.18	111.70
1	C	287	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	C	312	ASP	CB-CG-OD1	6.44	124.10	118.30
1	D	290	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	312	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	190	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	487	LEU	CB-CG-CD2	-5.81	101.12	111.00
1	C	190	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	446	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	290	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	358	ASP	CB-CG-OD1	5.12	122.91	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3725	38	0
1	B	3716	0	3736	57	0
1	C	3740	0	3752	55	0
1	D	3728	0	3738	43	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	53	0	31	0	0
2	D	53	0	31	1	0
3	A	33	0	27	0	0
3	B	33	0	27	2	0
3	C	33	0	27	2	0
3	D	33	0	27	2	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	364	0	0	6	0
6	B	343	0	0	12	0
6	C	350	0	0	11	0
6	D	370	0	0	7	0
All	All	16689	0	15183	189	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (189) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:480:LYS:HA	1:D:480:LYS:HE2	1.32	1.12
1:A:129:LEU:HD23	1:A:299:VAL:HG21	1.45	0.98
1:A:393:MET:HE2	1:A:414:LYS:HE3	1.48	0.95
1:A:485:GLU:HG2	1:A:486:LYS:HD2	1.55	0.86
1:C:94:LYS:HE2	6:C:3074:HOH:O	1.79	0.81
1:A:274:LYS:HD2	6:A:3205:HOH:O	1.79	0.81
1:D:101:GLU:HG3	6:D:3081:HOH:O	1.84	0.77
1:D:480:LYS:HA	1:D:480:LYS:CE	2.10	0.75
1:A:393:MET:CE	1:A:414:LYS:HE3	2.17	0.75
1:B:130:GLU:HB2	1:B:136:VAL:CG2	2.16	0.74
1:A:129:LEU:HD23	1:A:299:VAL:CG2	2.18	0.73
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.71	0.73
1:A:370:PRO:HD2	6:A:3298:HOH:O	1.88	0.73
1:C:318:ASN:H	1:C:318:ASN:HD22	1.36	0.73
1:D:486:LYS:HB2	6:D:3361:HOH:O	1.86	0.73
1:C:241:GLN:OE1	1:C:370:PRO:HG3	1.88	0.73
1:C:80:GLY:HA2	1:D:94:LYS:HG2	1.71	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:21:TRP:HZ2	3:C:1000:WP7:HBF	1.57	0.69
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.58	0.69
1:D:224:ASN:HD22	1:D:252:ASN:HD21	1.38	0.69
1:D:289:PRO:HG3	1:D:330:ASP:HB2	1.74	0.69
1:C:455:TYR:CZ	1:C:472:ARG:HD3	2.27	0.69
1:A:72:HIS:HD2	6:B:3036:HOH:O	1.75	0.68
1:C:380:GLU:O	1:C:384[B]:LYS:HD2	1.94	0.67
1:D:387:GLU:HA	1:D:480:LYS:HE3	1.78	0.65
1:B:218:THR:HG23	1:B:248:GLU:HG2	1.79	0.64
1:A:302:LYS:H	1:A:318:ASN:HD21	1.46	0.64
1:C:189:ARG:HA	1:C:212:PRO:HD2	1.80	0.64
1:A:318:ASN:H	1:A:318:ASN:HD22	1.47	0.63
1:A:4:ALA:HA	1:A:152:GLN:HG3	1.80	0.63
3:D:1000:WP7:CBF	3:D:1000:WP7:HBE1	2.28	0.63
1:C:318:ASN:HD22	1:C:318:ASN:N	1.97	0.62
1:A:295:GLN:HG3	6:A:3245:HOH:O	1.99	0.62
1:D:390:ALA:HB3	1:D:417:THR:OG1	1.99	0.62
1:B:464:SER:O	1:B:467:GLU:HB2	2.00	0.62
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.35	0.62
1:C:94:LYS:NZ	6:C:3076:HOH:O	2.32	0.62
1:D:13:GLY:HA3	2:D:998:FAD:H52A	1.81	0.62
1:B:130:GLU:HB2	1:B:136:VAL:HG23	1.82	0.61
1:A:302:LYS:H	1:A:318:ASN:ND2	1.99	0.61
1:C:331:ARG:HB3	6:C:3249:HOH:O	2.00	0.61
1:C:299:VAL:CG2	1:C:301:VAL:HG23	2.30	0.61
1:B:2:SER:C	1:B:3:LYS:HG3	2.21	0.60
1:D:387:GLU:HG3	1:D:480:LYS:HD2	1.83	0.60
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.84	0.59
1:D:129:LEU:HD23	1:D:299:VAL:HG21	1.82	0.59
1:B:129:LEU:HD23	1:B:299:VAL:HG21	1.84	0.59
1:B:266:LYS:N	1:B:266:LYS:HD2	2.17	0.59
1:D:302:LYS:H	1:D:318:ASN:HD21	1.50	0.59
1:D:318:ASN:H	1:D:318:ASN:HD22	1.50	0.59
1:B:313:GLU:HG3	6:B:3224:HOH:O	2.03	0.59
1:B:147:VAL:HG23	6:B:3104:HOH:O	2.02	0.58
1:D:302:LYS:H	1:D:318:ASN:ND2	2.02	0.58
1:C:274:LYS:HE2	6:C:3209:HOH:O	2.04	0.57
1:D:144:LYS:HE2	6:D:3125:HOH:O	2.05	0.57
1:B:162:SER:HB3	1:B:327:ASP:HB3	1.86	0.57
1:A:62:LEU:HD22	1:B:403:ILE:HD12	1.85	0.57
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.87	0.56
1:B:52:CYS:HB3	6:B:3004:HOH:O	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:104:LEU:HG	1:D:108:LYS:HE3	1.88	0.56
1:A:152:GLN:OE1	6:A:3128:HOH:O	2.18	0.56
1:D:227:LEU:HD12	1:D:238:VAL:HG11	1.86	0.56
1:C:240:LYS:HE2	6:C:3170:HOH:O	2.05	0.55
1:C:155:HIS:HB3	1:C:323:TYR:HE2	1.71	0.55
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.42	0.55
1:B:219:LEU:HD23	1:B:219:LEU:C	2.28	0.55
1:B:337:VAL:O	1:B:341:GLU:HG3	2.07	0.54
1:B:331:ARG:HB3	6:B:3240:HOH:O	2.07	0.54
1:D:211:LYS:NZ	6:D:3174:HOH:O	2.40	0.54
1:B:240:LYS:HD3	6:B:3057:HOH:O	2.06	0.54
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.90	0.53
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.44	0.53
1:D:400:MET:HG3	1:D:401:HIS:N	2.24	0.53
1:B:455:TYR:CZ	1:B:472:ARG:HD3	2.44	0.52
1:B:130:GLU:HB2	1:B:136:VAL:HG22	1.91	0.52
1:C:154:ASP:HB3	1:C:155:HIS:CD2	2.45	0.52
1:D:95:LEU:HD22	1:D:210:TYR:CZ	2.45	0.52
1:B:190[B]:ARG:HD3	1:B:216:LYS:HB3	1.91	0.51
1:B:410:LYS:HE2	6:B:3162:HOH:O	2.10	0.51
1:A:83:PHE:HB3	1:B:88:VAL:HG22	1.92	0.51
1:C:402:ASN:HA	1:C:407:LYS:HD3	1.92	0.51
1:C:449:ALA:HB2	1:D:447:LEU:HD11	1.93	0.51
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.74	0.51
1:C:480:LYS:HE3	6:C:3334:HOH:O	2.10	0.51
1:D:446:ARG:HD3	6:D:3335:HOH:O	2.09	0.51
1:C:302:LYS:H	1:C:318:ASN:ND2	2.09	0.50
3:D:1000:WP7:HBF	3:D:1000:WP7:HBE1	1.93	0.50
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.46	0.50
1:C:407:LYS:HB2	6:C:3292:HOH:O	2.10	0.50
1:C:75:GLU:HG2	1:C:404:SER:HB2	1.93	0.50
1:B:349:VAL:HG12	1:B:350:PHE:CD1	2.46	0.50
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.42	0.50
1:B:402:ASN:HA	1:B:407:LYS:HD3	1.92	0.50
1:A:189:ARG:HA	1:A:212:PRO:HD2	1.93	0.50
1:B:40:HIS:H	1:B:107:ASN:ND2	2.09	0.49
1:D:234:ILE:O	1:D:238:VAL:HG12	2.13	0.49
1:C:129:LEU:HD11	1:C:156:ILE:HG21	1.95	0.49
1:C:68:GLN:HG2	6:C:3049:HOH:O	2.13	0.49
1:C:198:PHE:HB2	1:C:366:VAL:HG13	1.94	0.49
1:A:218:THR:HG23	1:A:248:GLU:HG2	1.95	0.49
1:B:353:LYS:CB	6:B:3247:HOH:O	2.61	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:293:ASP:HB2	6:D:3234:HOH:O	2.12	0.48
1:B:353:LYS:HB3	6:B:3247:HOH:O	2.11	0.48
1:A:157:LEU:HD11	1:A:325:ILE:HG12	1.96	0.48
1:D:387:GLU:HG3	1:D:480:LYS:CD	2.44	0.48
1:A:69:TYR:O	1:A:73:LEU:HG	2.14	0.47
1:B:75:GLU:HB3	1:B:404:SER:HB2	1.96	0.47
1:C:476:TYR:CE2	1:C:483:LYS:HE3	2.50	0.47
1:D:40:HIS:H	1:D:107:ASN:ND2	2.12	0.47
1:B:455:TYR:CD2	1:B:472:ARG:HB3	2.50	0.47
1:C:480:LYS:CE	6:C:3334:HOH:O	2.63	0.47
1:C:89:LYS:HG2	1:C:90:ALA:N	2.30	0.47
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.97	0.47
1:C:148:LYS:C	1:C:149:GLU:HG2	2.34	0.47
1:C:325:ILE:O	1:C:328:ILE:HG22	2.14	0.47
3:C:1000:WP7:HAQ2	6:C:3348:HOH:O	2.14	0.47
1:C:318:ASN:ND2	1:C:318:ASN:N	2.64	0.46
1:C:94:LYS:HB3	1:C:94:LYS:HE3	1.60	0.46
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.81	0.46
1:C:218:THR:HG23	1:C:248:GLU:HG2	1.97	0.46
1:C:314:PHE:O	1:C:315:SER:HB2	2.15	0.46
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.98	0.46
1:C:227:LEU:HD12	1:C:238:VAL:HG11	1.98	0.46
1:B:129:LEU:HD23	1:B:299:VAL:CG2	2.46	0.46
1:B:321:ASN:HD22	1:B:321:ASN:N	2.13	0.46
1:B:250:MET:HE2	1:B:253:GLU:HG3	1.98	0.46
1:C:352:ASN:O	1:C:354:PRO:HD3	2.16	0.46
1:C:176:ILE:HB	1:C:180:GLU:HB2	1.96	0.46
1:C:72:HIS:HD2	6:C:3056:HOH:O	1.98	0.46
1:B:163:TRP:CG	1:B:164:PRO:HD2	2.51	0.45
1:D:455:TYR:CD2	1:D:472:ARG:HB3	2.50	0.45
1:A:4:ALA:CA	1:A:152:GLN:HG3	2.46	0.45
1:C:447:LEU:HD11	1:D:449:ALA:HB2	1.98	0.45
1:C:5:PHE:HE2	1:C:151:LEU:HD22	1.82	0.45
1:A:198:PHE:O	1:A:202:GLU:HG3	2.16	0.45
1:C:80:GLY:CA	1:D:94:LYS:HG2	2.45	0.45
1:D:190:ARG:NH2	1:D:279:ASP:OD1	2.48	0.45
1:A:304:THR:HG21	6:A:3250:HOH:O	2.16	0.45
1:D:40:HIS:H	1:D:107:ASN:HD21	1.65	0.45
1:B:8:VAL:HG23	1:B:153:ALA:HB2	1.99	0.45
1:B:18:GLU:OE1	3:B:1000:WP7:NBA	2.50	0.45
1:C:8:VAL:HG22	1:C:32:ALA:HB3	1.99	0.44
3:B:1000:WP7:HAP2	3:B:1000:WP7:HBC1	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:176:ILE:HB	1:D:180:GLU:HB2	2.00	0.44
1:A:437:ILE:HG12	1:A:465:ALA:HB2	2.00	0.44
1:B:190[A]:ARG:NH1	6:B:3132:HOH:O	2.30	0.43
1:D:157:LEU:HD11	1:D:325:ILE:HG12	2.01	0.43
1:C:370:PRO:HG2	1:C:430:LEU:HD11	2.01	0.43
1:C:484:MET:SD	1:C:488:PRO:HD3	2.58	0.43
1:B:45:TYR:CD1	1:B:179:ASN:HB3	2.54	0.43
1:A:155:HIS:HB3	1:A:323:TYR:HE2	1.82	0.43
1:D:319:VAL:HA	1:D:320:PRO:HD3	1.97	0.43
1:B:299:VAL:HG23	1:B:301:VAL:HG23	2.01	0.43
1:B:190[B]:ARG:CD	1:B:216:LYS:HB3	2.49	0.43
1:B:222:ARG:NH1	6:B:3180:HOH:O	2.51	0.43
1:B:40:HIS:H	1:B:107:ASN:HD21	1.67	0.43
1:B:388:LYS:HE2	1:B:388:LYS:HB3	1.86	0.43
1:B:349:VAL:HG12	1:B:350:PHE:CE1	2.54	0.42
1:B:76:SER:HB2	1:B:81:TRP:HB2	2.00	0.42
1:C:8:VAL:HG23	1:C:153:ALA:HB2	2.02	0.42
1:B:250:MET:CE	1:B:253:GLU:HG3	2.50	0.42
1:B:92:TRP:O	1:B:96:ILE:HG12	2.19	0.42
1:D:370:PRO:HD2	6:D:3301:HOH:O	2.20	0.42
1:A:171:GLY:HA3	1:A:258:VAL:O	2.20	0.42
1:B:2:SER:C	1:B:3:LYS:CG	2.88	0.42
1:C:453:ASP:CG	1:D:447:LEU:HD21	2.39	0.42
1:D:331:ARG:HG2	1:D:332:LEU:H	1.84	0.42
1:A:375:CYS:SG	1:A:445:LEU:HD22	2.59	0.42
1:B:389:VAL:HB	1:B:478:TYR:HB2	2.02	0.42
1:A:144:LYS:HB2	1:A:144:LYS:HE3	1.77	0.41
1:C:76:SER:HB2	1:C:81:TRP:HB2	2.02	0.41
1:C:1:MET:HA	1:C:1:MET:HE2	2.01	0.41
1:B:45:TYR:CG	1:B:179:ASN:HB3	2.55	0.41
1:B:353:LYS:CA	6:B:3247:HOH:O	2.68	0.41
1:C:221:TYR:CE2	1:C:223:ASN:HB2	2.56	0.41
1:C:302:LYS:HD3	1:C:303:LEU:O	2.21	0.41
1:C:157:LEU:HD11	1:C:325:ILE:HG12	2.01	0.41
1:D:17:LEU:HA	1:D:17:LEU:HD23	1.98	0.41
1:D:485:GLU:O	1:D:486:LYS:HG2	2.20	0.41
1:C:327:ASP:OD1	1:C:333:MET:HA	2.20	0.41
1:A:68:GLN:NE2	6:A:3049:HOH:O	2.53	0.41
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.83	0.41
1:A:174:HIS:CE1	1:A:260:LEU:HG	2.56	0.41
1:B:461:HIS:HA	1:B:462:PRO:HA	1.92	0.40
1:B:190[A]:ARG:HB2	1:B:190[A]:ARG:HE	1.72	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.55	0.40
1:C:5:PHE:CE2	1:C:151:LEU:HD22	2.55	0.40
1:D:167:PRO:HD3	1:D:285:ILE:CD1	2.51	0.40
1:B:93:LYS:NZ	1:B:186:GLU:OE2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/495 (98%)	472 (97%)	12 (2%)	3 (1%)	33	28
1	B	488/495 (99%)	473 (97%)	15 (3%)	0	100	100
1	C	491/495 (99%)	475 (97%)	15 (3%)	1 (0%)	56	57
1	D	489/495 (99%)	473 (97%)	14 (3%)	2 (0%)	43	39
All	All	1955/1980 (99%)	1893 (97%)	56 (3%)	6 (0%)	50	49

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LYS
1	C	480	LYS
1	D	480	LYS
1	A	213	PRO
1	D	55	VAL
1	A	55	VAL

### 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	402/407 (99%)	385 (96%)	17 (4%)	40	38
1	B	402/407 (99%)	387 (96%)	15 (4%)	45	45
1	C	405/407 (100%)	383 (95%)	22 (5%)	31	27
1	D	404/407 (99%)	387 (96%)	17 (4%)	40	38
All	All	1613/1628 (99%)	1542 (96%)	71 (4%)	39	36

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	CYS
1	A	60	LYS
1	A	89	LYS
1	A	99	LYS
1	A	101	GLU
1	A	152	GLN
1	A	213	PRO
1	A	224	ASN
1	A	237	GLU
1	A	238	VAL
1	A	266	LYS
1	A	306	LYS
1	A	318	ASN
1	A	394	SER
1	A	400	MET
1	A	480	LYS
1	A	485	GLU
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	216	LYS
1	B	224	ASN
1	B	292	ASN
1	B	306	LYS
1	B	313	GLU
1	B	321	ASN
1	B	385	GLU
1	B	400	MET
1	B	462	PRO
1	B	467	GLU
1	B	485	GLU
1	B	487	LEU
1	C	1	MET

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Mol	Chain	Res	Type
1	C	30	ARG
1	C	39	SER
1	C	57	CYS
1	C	60	LYS
1	C	99	LYS
1	C	129	LEU
1	C	150	ARG
1	C	152	GLN
1	C	154	ASP
1	C	189	ARG
1	C	228	ARG
1	C	238	VAL
1	C	259	SER
1	C	260	LEU
1	C	262	THR
1	C	306	LYS
1	C	318	ASN
1	C	335	THR
1	C	400	MET
1	C	446	ARG
1	C	480	LYS
1	D	30	ARG
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	94	LYS
1	D	99	LYS
1	D	186	GLU
1	D	260	LEU
1	D	266	LYS
1	D	274	LYS
1	D	318	ASN
1	D	321	ASN
1	D	335	THR
1	D	400	MET
1	D	470	SER
1	D	480	LYS
1	D	487	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	72	HIS
1	A	152	GLN
1	A	318	ASN
1	B	107	ASN
1	B	224	ASN
1	B	310	GLN
1	B	321	ASN
1	C	72	HIS
1	C	107	ASN
1	C	152	GLN
1	C	318	ASN
1	D	107	ASN
1	D	152	GLN
1	D	224	ASN
1	D	295	GLN
1	D	318	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 19 are monoatomic - leaving 8 for Mogul analysis.

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
3	WP7	A	1000	-	37,37,37	1.76	7 (18%)	51,52,52	1.90	10 (19%)
2	FAD	A	998	-	58,58,58	1.26	7 (12%)	85,89,89	2.13	12 (14%)
3	WP7	B	1000	-	37,37,37	2.17	9 (24%)	51,52,52	1.89	12 (23%)
2	FAD	B	998	-	58,58,58	1.22	8 (13%)	85,89,89	2.25	19 (22%)
3	WP7	C	1000	-	37,37,37	1.68	6 (16%)	51,52,52	1.84	13 (25%)
2	FAD	C	998	-	58,58,58	1.08	4 (6%)	85,89,89	1.75	14 (16%)
3	WP7	D	1000	-	37,37,37	2.24	10 (27%)	51,52,52	1.99	16 (31%)
2	FAD	D	998	-	58,58,58	1.48	10 (17%)	85,89,89	2.46	28 (32%)

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
3	WP7	A	1000	-	-	0/15/43/43	0/3/5/5
2	FAD	A	998	-	-	0/34/50/50	0/1/6/6
3	WP7	B	1000	-	-	0/15/43/43	0/3/5/5
2	FAD	B	998	-	-	0/34/50/50	0/1/6/6
3	WP7	C	1000	-	-	0/15/43/43	0/3/5/5
2	FAD	C	998	-	-	0/34/50/50	0/1/6/6
3	WP7	D	1000	-	-	0/15/43/43	0/3/5/5
2	FAD	D	998	-	-	0/34/50/50	0/1/6/6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	WP7	CBB-NBA	6.81	1.41	1.29
3	B	1000	WP7	CBB-NBA	6.37	1.41	1.29
3	D	1000	WP7	CBB-NAO	6.07	1.45	1.35
3	B	1000	WP7	CAN-NAO	5.36	1.51	1.48
3	D	1000	WP7	CBC-CBB	4.65	1.57	1.49
3	C	1000	WP7	CBC-CBB	4.38	1.57	1.49
3	C	1000	WP7	CBB-NAO	4.37	1.42	1.35
3	B	1000	WP7	CBB-NAO	4.31	1.42	1.35
3	C	1000	WP7	CBB-NBA	4.23	1.37	1.29
2	A	998	FAD	C1'-C2'	4.14	1.55	1.51
3	A	1000	WP7	CBB-NAO	3.98	1.41	1.35
2	D	998	FAD	C2A-N3A	3.91	1.39	1.32
3	B	1000	WP7	CAU-CAT	3.88	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	WP7	CAN-NAO	3.87	1.50	1.48
3	A	1000	WP7	CBC-CBB	3.70	1.55	1.49
3	B	1000	WP7	CBC-CBB	3.70	1.55	1.49
3	A	1000	WP7	CAH-NAS	3.58	1.53	1.47
2	B	998	FAD	C5X-N5	3.56	1.40	1.35
3	D	1000	WP7	CAU-CAT	3.51	1.58	1.50
2	D	998	FAD	C2A-N1A	3.46	1.40	1.33
2	D	998	FAD	C10-N1	3.43	1.41	1.35
3	A	1000	WP7	CBE-NAS	3.38	1.53	1.47
3	B	1000	WP7	CBE-NAS	3.25	1.52	1.47
2	D	998	FAD	C5X-N5	3.24	1.40	1.35
3	B	1000	WP7	CAE-CAN	3.14	1.56	1.52
3	B	1000	WP7	CAH-NAS	2.98	1.52	1.47
3	B	1000	WP7	CAL-CAK	2.89	1.43	1.38
3	A	1000	WP7	CAU-CAT	2.85	1.56	1.50
3	C	1000	WP7	CAU-CAT	2.85	1.56	1.50
2	B	998	FAD	C2A-N3A	2.77	1.37	1.32
2	C	998	FAD	C2A-N1A	2.76	1.39	1.33
2	A	998	FAD	C4A-N9A	-2.75	1.33	1.37
2	A	998	FAD	C2A-N1A	2.74	1.39	1.33
2	D	998	FAD	C2B-C1B	-2.70	1.49	1.53
3	A	1000	WP7	CBB-NBA	2.69	1.34	1.29
2	C	998	FAD	C6-C5X	-2.62	1.38	1.41
3	D	1000	WP7	CAE-CAN	2.58	1.55	1.52
2	C	998	FAD	C2A-N3A	2.56	1.37	1.32
3	C	1000	WP7	CAM-CAN	2.55	1.54	1.52
2	D	998	FAD	PA-O3P	2.53	1.64	1.59
3	C	1000	WP7	CAL-CAK	2.48	1.42	1.38
2	A	998	FAD	C2-N3	2.42	1.42	1.37
3	D	1000	WP7	CAM-CAN	2.41	1.54	1.52
2	B	998	FAD	C5'-C4'	2.34	1.55	1.51
2	D	998	FAD	C4-N3	2.33	1.41	1.37
3	D	1000	WP7	CAP-NAO	2.33	1.50	1.46
3	A	1000	WP7	CAE-CAN	2.29	1.55	1.52
2	A	998	FAD	P-O3P	2.29	1.64	1.59
3	D	1000	WP7	CAH-NAS	2.28	1.51	1.47
2	A	998	FAD	C1'-N10	2.23	1.50	1.48
2	D	998	FAD	O5B-C5B	-2.23	1.35	1.44
2	C	998	FAD	C5X-N5	2.20	1.38	1.35
2	A	998	FAD	C5X-N5	2.16	1.38	1.35
2	D	998	FAD	C2-N3	2.16	1.41	1.37
2	B	998	FAD	C2A-N1A	2.13	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	FAD	C6-C7	2.11	1.43	1.37
3	D	1000	WP7	CAK-CLA	-2.08	1.69	1.74
2	B	998	FAD	C1'-N10	2.05	1.50	1.48
2	D	998	FAD	O4B-C1B	2.03	1.44	1.41
2	B	998	FAD	P-O3P	-2.03	1.56	1.59
2	B	998	FAD	C8-C7	-2.01	1.35	1.40

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	FAD	N3A-C2A-N1A	-12.47	118.28	128.71
2	A	998	FAD	N3A-C2A-N1A	-11.67	118.96	128.71
2	D	998	FAD	C4B-O4B-C1B	-10.55	98.29	109.75
2	C	998	FAD	N3A-C2A-N1A	-9.87	120.46	128.71
2	D	998	FAD	N3A-C2A-N1A	-9.28	120.95	128.71
2	B	998	FAD	O4B-C1B-N9A	-6.08	102.79	108.44
2	D	998	FAD	O3B-C3B-C4B	-5.85	93.84	111.08
2	A	998	FAD	O4B-C1B-N9A	-5.60	103.23	108.44
3	D	1000	WP7	OAV-CAW-CBG	-5.44	107.28	111.53
3	A	1000	WP7	OAV-CAW-CBG	-5.33	107.36	111.53
2	B	998	FAD	C1'-N10-C9A	5.07	123.80	118.87
3	B	1000	WP7	OAV-CAW-CBG	-5.05	107.58	111.53
2	D	998	FAD	C4X-N5-C5X	5.02	122.33	116.69
3	A	1000	WP7	CBE-NAS-CAH	4.95	121.96	112.52
3	D	1000	WP7	CAL-CAK-CLA	-4.94	113.04	119.14
2	D	998	FAD	O2A-PA-O5B	4.93	133.35	108.51
2	D	998	FAD	C4X-C10-N10	-4.92	118.05	120.51
3	B	1000	WP7	CBC-CBB-NAO	4.89	123.70	117.85
2	A	998	FAD	C5X-C9A-N10	4.89	121.61	116.80
2	D	998	FAD	C4A-C5A-N7A	-4.75	105.45	109.52
3	D	1000	WP7	CBC-CBB-NAO	4.72	123.49	117.85
3	C	1000	WP7	OAV-CAW-CBG	-4.62	107.92	111.53
3	C	1000	WP7	CAZ-NBA-CBB	4.42	123.96	118.38
2	A	998	FAD	C2-N1-C10	4.39	119.40	114.98
2	B	998	FAD	C2-N1-C10	4.36	119.37	114.98
2	B	998	FAD	C4X-N5-C5X	4.28	121.50	116.69
3	C	1000	WP7	CBC-CBB-NAO	4.21	122.88	117.85
2	A	998	FAD	C4X-N5-C5X	4.18	121.39	116.69
2	A	998	FAD	C2A-N1A-C6A	4.10	126.17	118.77
2	B	998	FAD	C4A-C5A-N7A	-4.03	106.07	109.52
3	B	1000	WP7	CBE-NAS-CAH	3.98	120.10	112.52
3	D	1000	WP7	CAZ-NBA-CBB	3.97	123.39	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1000	WP7	CAW-OAV-CAU	-3.95	105.59	106.42
3	B	1000	WP7	NAO-CBB-NBA	-3.87	118.38	123.33
3	B	1000	WP7	CAU-CAT-NAS	3.87	126.35	119.74
2	B	998	FAD	N3A-C4A-N9A	3.85	132.38	125.43
2	A	998	FAD	C4X-C10-N1	-3.78	118.95	122.73
2	A	998	FAD	C4-N3-C2	-3.77	117.65	125.39
3	B	1000	WP7	CAZ-NBA-CBB	3.76	123.12	118.38
2	D	998	FAD	O4B-C1B-N9A	-3.71	104.99	108.44
3	D	1000	WP7	NAO-CBB-NBA	-3.70	118.61	123.33
3	A	1000	WP7	CBC-CBB-NAO	3.67	122.24	117.85
2	C	998	FAD	N3A-C4A-N9A	3.64	132.00	125.43
3	B	1000	WP7	OAI-CAT-NAS	-3.63	115.57	122.33
3	C	1000	WP7	NAO-CBB-NBA	-3.57	118.77	123.33
2	B	998	FAD	C4X-C10-N1	-3.51	119.22	122.73
2	C	998	FAD	C1'-N10-C9A	3.46	122.24	118.87
3	A	1000	WP7	CAQ-CAP-NAO	-3.45	106.39	112.08
3	C	1000	WP7	CAQ-NAR-CBD	3.44	120.20	111.32
3	C	1000	WP7	CAE-CAN-NAO	-3.43	106.33	111.54
2	A	998	FAD	C9A-N10-C10	-3.43	118.40	121.77
2	D	998	FAD	N3A-C4A-N9A	3.43	131.62	125.43
3	A	1000	WP7	CAE-CAN-NAO	-3.39	106.39	111.54
3	C	1000	WP7	CBD-CBE-NAS	-3.37	102.42	110.58
2	C	998	FAD	C2-N1-C10	3.36	118.36	114.98
2	C	998	FAD	C4A-C5A-N7A	-3.28	106.71	109.52
3	D	1000	WP7	CAY-CAX-CAK	-3.23	115.61	119.22
2	D	998	FAD	O4B-C4B-C5B	3.20	120.80	109.36
2	B	998	FAD	C4'-C3'-C2'	-3.20	106.02	113.25
3	D	1000	WP7	CAM-CAZ-NBA	-3.16	118.93	122.22
3	A	1000	WP7	CAP-CAQ-NAR	-3.15	104.98	113.28
2	C	998	FAD	C9A-N10-C10	-3.15	118.68	121.77
3	D	1000	WP7	OAI-CAT-NAS	-3.08	116.60	122.33
3	A	1000	WP7	CAW-OAV-CAU	-3.06	105.78	106.42
3	C	1000	WP7	CAQ-CAP-NAO	-3.05	107.04	112.08
3	B	1000	WP7	CAQ-CAP-NAO	-3.03	107.08	112.08
2	D	998	FAD	C4-N3-C2	-2.97	119.29	125.39
2	B	998	FAD	C2A-N3A-C4A	2.97	122.46	114.01
2	C	998	FAD	C4X-C10-N10	2.94	121.98	120.51
2	D	998	FAD	P-O3P-PA	2.87	140.09	131.68
2	D	998	FAD	C2-N1-C10	2.86	117.86	114.98
2	B	998	FAD	N7A-C8A-N9A	-2.79	106.47	114.36
2	A	998	FAD	C4-C4X-C10	2.77	121.42	116.95
3	C	1000	WP7	CBD-NAR-CAG	2.77	115.73	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	FAD	C5A-C4A-N3A	-2.72	119.77	125.70
2	B	998	FAD	C4-C4X-C10	2.71	121.32	116.95
3	C	1000	WP7	CAY-CAZ-CAM	2.70	121.97	119.56
2	D	998	FAD	C6-C5X-N5	2.69	122.11	118.97
2	D	998	FAD	N7A-C8A-N9A	-2.69	106.74	114.36
2	A	998	FAD	C9A-C5X-N5	-2.69	118.24	122.37
2	B	998	FAD	O3'-C3'-C2'	2.69	115.53	108.74
3	B	1000	WP7	CAE-CAN-NAO	-2.67	107.48	111.54
3	B	1000	WP7	CAP-CAQ-NAR	-2.66	106.27	113.28
2	D	998	FAD	C8A-N7A-C5A	2.65	111.81	103.58
3	A	1000	WP7	NAO-CBB-NBA	-2.65	119.94	123.33
2	B	998	FAD	C8A-N7A-C5A	2.59	111.60	103.58
2	C	998	FAD	C5A-C4A-N3A	-2.58	120.08	125.70
2	D	998	FAD	C9A-C5X-N5	-2.57	118.43	122.37
3	D	1000	WP7	CAW-OAV-CAU	2.56	106.96	106.42
3	C	1000	WP7	CAE-CAN-CAM	-2.52	108.09	112.54
2	C	998	FAD	C4-N3-C2	-2.52	120.22	125.39
2	D	998	FAD	C6A-C5A-C4A	2.51	121.86	117.25
2	B	998	FAD	C1'-N10-C10	-2.51	115.61	119.17
2	D	998	FAD	C4-C4X-C10	2.48	120.95	116.95
3	D	1000	WP7	CBE-NAS-CAH	2.48	117.24	112.52
3	A	1000	WP7	CAK-CAL-CAM	-2.46	117.32	120.08
3	A	1000	WP7	CAQ-NAR-CAG	2.46	117.68	111.32
3	B	1000	WP7	CAE-CAN-CAM	-2.45	108.21	112.54
2	D	998	FAD	O5B-PA-O1A	-2.43	99.84	109.37
2	D	998	FAD	O4'-C4'-C5'	-2.43	105.14	110.12
2	D	998	FAD	C5X-C9A-N10	2.40	119.17	116.80
2	D	998	FAD	O3P-PA-O5B	-2.40	92.68	103.41
3	D	1000	WP7	CAQ-NAR-CAG	2.36	117.41	111.32
2	D	998	FAD	C1B-N9A-C4A	-2.32	122.63	126.64
2	A	998	FAD	C5A-C6A-N6A	2.31	125.95	120.72
2	C	998	FAD	C5X-C9A-N10	2.28	119.05	116.80
3	D	1000	WP7	CAE-CAN-NAO	-2.25	108.12	111.54
2	C	998	FAD	C5B-C4B-C3B	-2.22	106.32	115.21
2	B	998	FAD	C3B-C2B-C1B	2.20	104.36	100.91
3	D	1000	WP7	CAU-CAT-NAS	2.19	123.48	119.74
3	C	1000	WP7	CAM-CAZ-NBA	-2.18	119.96	122.22
2	B	998	FAD	C4-N3-C2	-2.18	120.92	125.39
2	D	998	FAD	C4X-C10-N1	-2.17	120.56	122.73
2	C	998	FAD	C8A-N7A-C5A	2.17	110.30	103.58
3	B	1000	WP7	CAL-CAK-CLA	2.16	121.81	119.14
2	D	998	FAD	C5A-C4A-N3A	-2.14	121.03	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1000	WP7	CAQ-CAP-NAO	-2.14	108.55	112.08
2	C	998	FAD	C2B-C1B-N9A	2.14	118.76	113.27
2	C	998	FAD	N7A-C8A-N9A	-2.13	108.34	114.36
2	D	998	FAD	C8A-N9A-C4A	2.10	108.50	106.90
2	D	998	FAD	N1-C10-N10	2.06	121.39	115.97
3	D	1000	WP7	CAX-CAK-CLA	2.06	122.74	119.34
3	D	1000	WP7	CAE-CAN-CAM	2.05	116.17	112.54
2	B	998	FAD	C4B-O4B-C1B	-2.05	107.53	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	489/495 (98%)	-0.36	3 (0%) 86 90	7, 16, 29, 40	0
1	B	487/495 (98%)	-0.11	8 (1%) 68 72	9, 20, 37, 48	0
1	C	492/495 (99%)	-0.11	9 (1%) 65 69	8, 20, 41, 53	0
1	D	490/495 (98%)	-0.30	8 (1%) 68 72	8, 17, 29, 56	0
All	All	1958/1980 (98%)	-0.22	28 (1%) 72 76	7, 18, 37, 56	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	487	LEU	5.2
1	D	488	PRO	5.0
1	B	352	ASN	3.7
1	C	384[A]	LYS	3.2
1	C	352	ASN	3.1
1	D	480	LYS	3.0
1	C	481	GLY	2.9
1	A	305	PRO	2.9
1	C	486	LYS	2.8
1	D	481	GLY	2.7
1	C	30	ARG	2.7
1	B	488	PRO	2.7
1	C	488	PRO	2.6
1	A	306	LYS	2.6
1	C	132	LYS	2.4
1	D	478	TYR	2.4
1	D	305	PRO	2.4
1	D	479	VAL	2.4
1	B	2	SER	2.3
1	A	352	ASN	2.3
1	B	321	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	135	VAL	2.3
1	B	478	TYR	2.2
1	B	384	LYS	2.2
1	C	487	LEU	2.1
1	C	381	VAL	2.1
1	B	322	ILE	2.0
1	D	387	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	NA	D	1492	1/1	0.15	4.42	29,29,29,29	0
5	NA	B	2005	1/1	0.19	3.62	32,32,32,32	0
3	WP7	A	1000	33/33	0.14	2.39	12,20,61,62	0
3	WP7	D	1000	33/33	0.13	1.94	10,18,61,62	0
3	WP7	C	1000	33/33	0.15	1.69	25,32,68,68	0
3	WP7	B	1000	33/33	0.14	1.45	21,27,72,72	0
2	FAD	D	998	53/53	0.10	0.78	2,10,15,23	0
2	FAD	A	998	53/53	0.10	0.40	3,9,12,14	0
4	CL	D	1490	1/1	0.09	-0.28	16,16,16,16	0
2	FAD	B	998	53/53	0.10	-0.29	7,16,30,31	0
4	CL	B	2002	1/1	0.09	-0.30	15,15,15,15	0
2	FAD	C	998	53/53	0.10	-0.32	7,17,23,25	0
4	CL	A	1490	1/1	0.09	-0.39	32,32,32,32	0
4	CL	C	1490	1/1	0.07	-0.55	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	1491	1/1	0.11	-0.83	19,19,19,19	0
4	CL	A	1488	1/1	0.06	-1.06	15,15,15,15	0
5	NA	A	1492	1/1	0.07	-1.17	28,28,28,28	0
4	CL	A	1489	1/1	0.05	-1.47	22,22,22,22	0
4	CL	B	2003	1/1	0.06	-1.59	34,34,34,34	0
4	CL	D	1489	1/1	0.04	-1.65	28,28,28,28	0
4	CL	D	1491	1/1	0.08	-1.70	33,33,33,33	0
5	NA	C	1493	1/1	0.08	-1.77	19,19,19,19	0
5	NA	D	1493	1/1	0.04	-1.86	19,19,19,19	0
4	CL	C	1491	1/1	0.04	-1.92	34,34,34,34	0
5	NA	C	1492	1/1	0.07	-2.37	44,44,44,44	0
4	CL	B	2001	1/1	0.05	-2.69	20,20,20,20	0
5	NA	B	2004	1/1	0.06	-6.26	30,30,30,30	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.