



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:48 PM GMT

PDB ID : 2WPF  
Title : TRYPANOSOMA BRUCEI TRYPANOTHIONE REDUCTASE IN COM-  
PLEX WITH 3,4-DIHYDROQUINAZOLINEINHIBITOR (DDD00085762)  
Authors : Alphey, M.S.; Patterson, S.; Fairlamb, A.H.  
Deposited on : 2009-08-06  
Resolution : 1.90 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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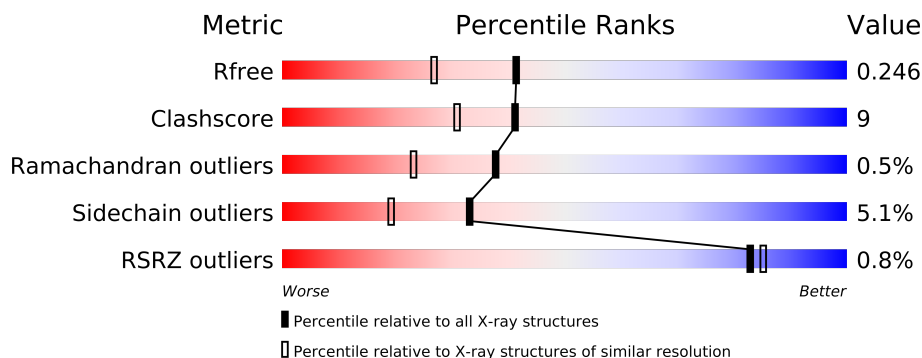
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	WPF	A	1000	-	X
3	WPF	B	1000	-	X
3	WPF	C	1000	-	X
3	WPF	D	1000	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16503 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	490	Total	C	N	O	S	0	2	0
			3733	2374	636	702	21			
1	B	487	Total	C	N	O	S	0	2	0
			3702	2353	631	699	19			
1	C	487	Total	C	N	O	S	0	3	0
			3716	2364	630	703	19			
1	D	491	Total	C	N	O	S	0	2	0
			3737	2376	635	706	20			

There are 12 discrepancies between the modelled and reference sequences:

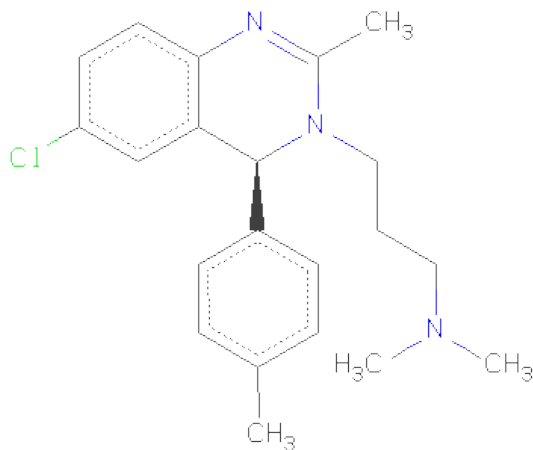
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P39051
A	-1	SER	-	EXPRESSION TAG	UNP P39051
A	0	HIS	-	EXPRESSION TAG	UNP P39051
B	-2	GLY	-	EXPRESSION TAG	UNP P39051
B	-1	SER	-	EXPRESSION TAG	UNP P39051
B	0	HIS	-	EXPRESSION TAG	UNP P39051
C	-2	GLY	-	EXPRESSION TAG	UNP P39051
C	-1	SER	-	EXPRESSION TAG	UNP P39051
C	0	HIS	-	EXPRESSION TAG	UNP P39051
D	-2	GLY	-	EXPRESSION TAG	UNP P39051
D	-1	SER	-	EXPRESSION TAG	UNP P39051
D	0	HIS	-	EXPRESSION TAG	UNP P39051

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



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 3-[(4S)-6-CHLORO-2-METHYL-4-(4-METHYLPHENYL)QUINAZOLI N-3(4H)-YL]-N,N-DIMETHYLPROPAN-1-AMINE (three-letter code: WPF) (formula: C<sub>21</sub>H<sub>26</sub>ClN<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	21	1	3		
3	B	1	Total	C	Cl	N	0	0
			25	21	1	3		
3	C	1	Total	C	Cl	N	0	0
			25	21	1	3		
3	D	1	Total	C	Cl	N	0	0
			25	21	1	3		

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

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

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Br	0	0
			1	1		
5	D	2	Total	Br	0	0
			2	2		

- Molecule 6 is water.

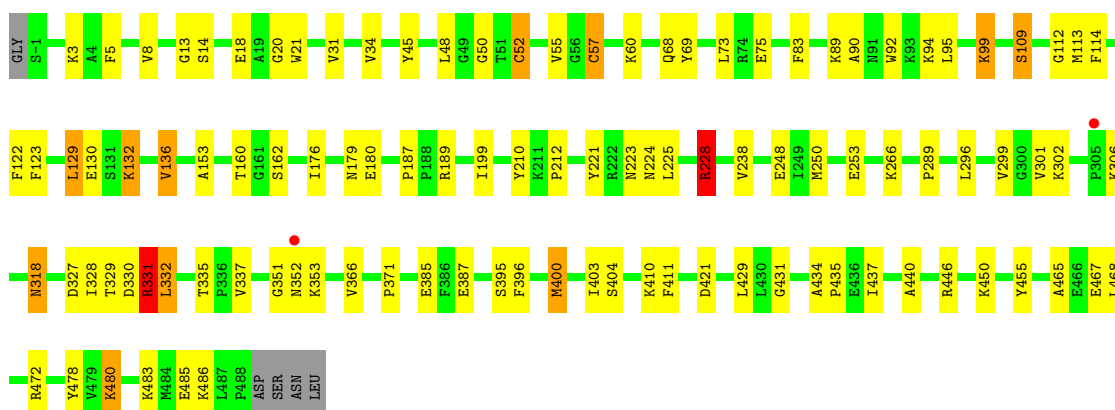
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	374	Total	O	0	0
			374	374		
6	B	290	Total	O	0	0
			290	290		
6	C	282	Total	O	0	0
			282	282		
6	D	347	Total	O	0	0
			347	347		

### 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.

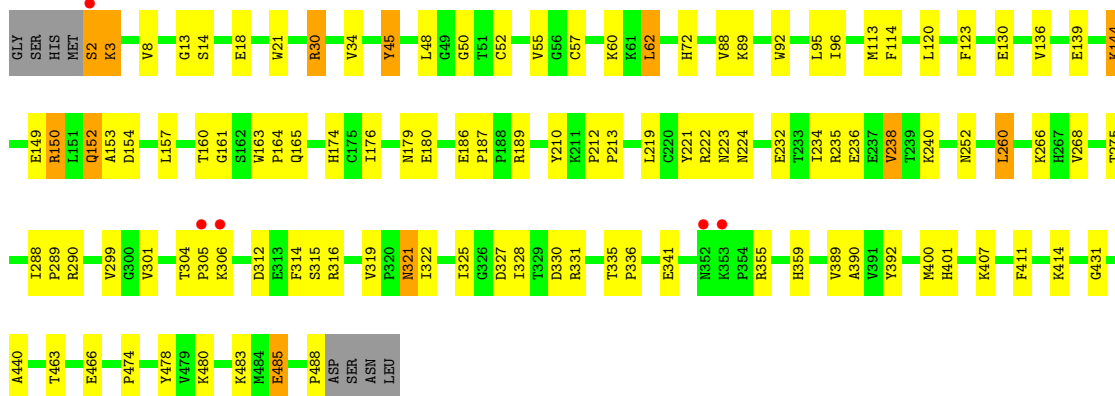
#### • Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



#### • Molecule 1: TRYPANOTHIONE REDUCTASE

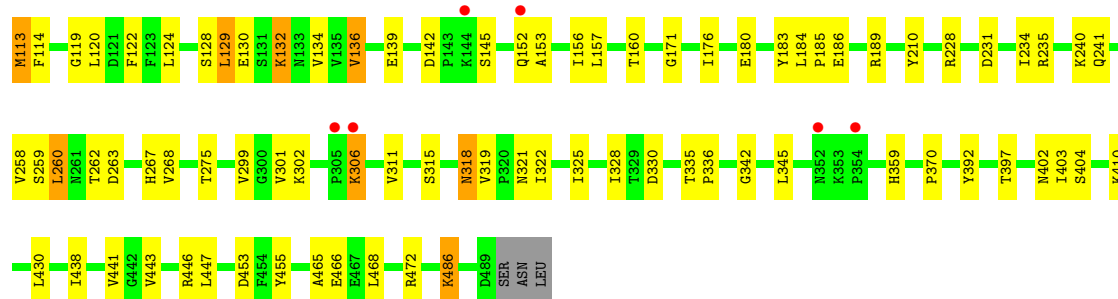
Chain B:



#### • Molecule 1: TRYPANOTHIONE REDUCTASE

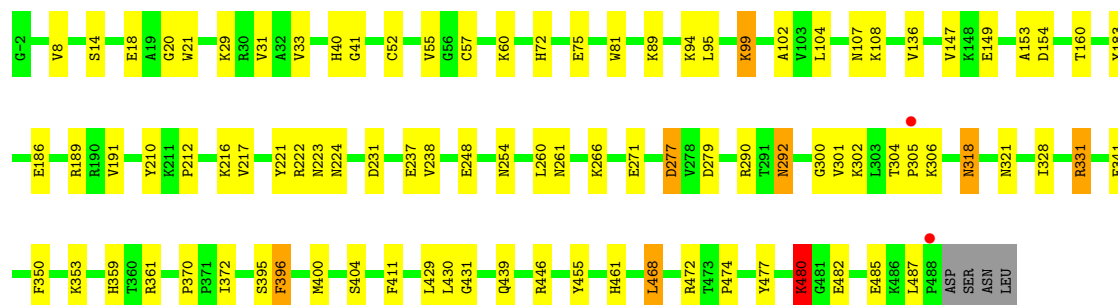
Chain C:





• 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, $\alpha$ , $\beta$ , $\gamma$	99.82Å 62.76Å 167.44Å 90.00° 98.13° 90.00°	Depositor
Resolution (Å)	19.89 – 1.90 19.89 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.89-1.90) 99.4 (19.89-1.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.185 , 0.247 0.185 , 0.246	Depositor DCC
$R_{free}$ test set	8048 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 33.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 160960 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16503	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.34% 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: WPF, BR, 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	1.10	3/3818 (0.1%)	1.00	3/5178 (0.1%)
1	B	0.98	1/3785 (0.0%)	0.93	7/5135 (0.1%)
1	C	0.97	2/3803 (0.1%)	0.92	4/5161 (0.1%)
1	D	1.04	1/3822 (0.0%)	0.95	6/5184 (0.1%)
All	All	1.02	7/15228 (0.0%)	0.95	20/20658 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ARG	CG-CD	6.56	1.68	1.51
1	C	240	LYS	CD-CE	5.77	1.65	1.51
1	A	366	VAL	CB-CG1	5.28	1.64	1.52
1	C	240	LYS	CE-NZ	5.23	1.62	1.49
1	A	136	VAL	CB-CG2	-5.11	1.42	1.52
1	D	33	VAL	CB-CG2	-5.10	1.42	1.52
1	B	238	VAL	CB-CG1	-5.09	1.42	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331[A]	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	331[B]	ARG	NE-CZ-NH2	-9.95	115.33	120.30
1	A	228	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	290	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	B	312	ASP	CB-CG-OD1	5.85	123.57	118.30
1	B	260	LEU	CA-CB-CG	5.71	128.44	115.30
1	D	361	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	D	154	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	279	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	C	453	ASP	CB-CG-OD1	-5.34	113.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	LEU	CB-CG-CD1	-5.33	101.95	111.00
1	C	260	LEU	CB-CG-CD2	5.26	119.94	111.00
1	B	266	LYS	CD-CE-NZ	-5.21	99.72	111.70
1	D	260	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	488	PRO	N-CA-CB	5.13	109.45	103.30
1	D	468	LEU	CB-CG-CD2	5.12	119.70	111.00
1	C	235	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	D	279	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	312	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	263	ASP	CB-CG-OD1	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	3733	0	3750	74	0
1	B	3702	0	3701	75	0
1	C	3716	0	3725	76	0
1	D	3737	0	3747	61	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	25	0	26	4	0
3	B	25	0	26	3	0
3	C	25	0	26	8	0
3	D	25	0	26	3	0
4	A	3	0	0	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	B	1	0	0	0	0
5	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	374	0	0	14	0
6	B	290	0	0	10	0
6	C	282	0	0	5	0
6	D	347	0	0	8	0
All	All	16503	0	15151	278	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 9.

All (278) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2:SER:O	1:B:3:LYS:HG2	1.61	0.99
1:B:8:VAL:HG23	1:B:153:ALA:HB2	1.51	0.91
1:B:130:GLU:HB2	1:B:136:VAL:HG23	1.53	0.91
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.01	0.89
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.46	0.80
1:A:485:GLU:HG2	1:A:486:LYS:HD3	1.65	0.79
1:C:241:GLN:OE1	1:C:370:PRO:HG3	1.84	0.78
1:D:331:ARG:HG3	1:D:331:ARG:HH11	1.49	0.78
3:A:1000:WPF:HAX1	6:A:2023:HOH:O	1.83	0.77
1:A:331[A]:ARG:NH2	6:A:2278:HOH:O	2.18	0.76
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.67	0.75
1:D:318:ASN:H	1:D:318:ASN:HD22	1.35	0.75
1:D:331:ARG:CG	1:D:331:ARG:HH11	1.99	0.74
1:B:30:ARG:HH21	1:B:30:ARG:HG3	1.53	0.73
1:B:174:HIS:HD2	6:B:2054:HOH:O	1.69	0.72
1:A:52[A]:CYS:HB3	6:A:2017:HOH:O	1.90	0.72
1:B:139:GLU:HG3	6:B:2085:HOH:O	1.90	0.72
1:C:302:LYS:H	1:C:318:ASN:ND2	1.88	0.71
1:D:429:LEU:HD21	1:D:468:LEU:HD21	1.71	0.71
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.72	0.71
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.27	0.69
1:C:142:ASP:O	1:C:145:SER:OG	2.11	0.69
1:B:224[A]:ASN:HD22	1:B:252:ASN:HD21	1.41	0.69
1:C:157:LEU:HD11	1:C:325:ILE:HG12	1.75	0.69
1:A:21:TRP:CD1	3:A:1000:WPF:HAX3	2.28	0.68
1:D:136:VAL:HG23	1:D:147:VAL:HG13	1.76	0.68
1:D:72:HIS:HE1	6:D:2047:HOH:O	1.75	0.68
1:B:130:GLU:HB2	1:B:136:VAL:CG2	2.24	0.67
6:A:2060:HOH:O	1:B:72:HIS:HD2	1.78	0.66
1:B:485:GLU:HG3	1:B:485:GLU:O	1.96	0.65
1:B:8:VAL:HG23	1:B:153:ALA:CB	2.24	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:314:PHE:O	1:B:315:SER:HB2	1.97	0.64
1:A:485:GLU:HG2	1:A:486:LYS:CD	2.28	0.64
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.79	0.64
1:A:318:ASN:H	1:A:318:ASN:HD22	1.46	0.63
1:C:319:VAL:HG11	1:C:322:ILE:HD12	1.81	0.63
1:C:110:TYR:OH	3:C:1000:WPF:HAJ	1.99	0.63
1:D:21:TRP:CD1	3:D:1000:WPF:HAX3	2.33	0.63
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.62	0.63
1:D:237:GLU:HB3	1:D:430:LEU:CD2	2.29	0.62
1:B:319:VAL:HG11	1:B:322:ILE:HD12	1.80	0.62
1:B:299:VAL:CG2	1:B:301:VAL:HG23	2.30	0.62
1:A:446:ARG:NE	6:A:2338:HOH:O	2.30	0.62
1:C:319:VAL:CG1	1:C:322:ILE:HD12	2.30	0.61
1:D:304:THR:HB	1:D:305:PRO:HD2	1.82	0.61
1:D:370:PRO:HG2	6:D:2300:HOH:O	2.01	0.61
1:B:8:VAL:CG2	1:B:153:ALA:HB2	2.29	0.61
1:D:238:VAL:HG21	1:D:372:ILE:HD11	1.82	0.60
1:C:113:MET:HB2	3:C:1000:WPF:HAA1	1.83	0.60
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.82	0.59
1:D:189:ARG:HA	1:D:212:PRO:HD2	1.84	0.59
1:A:434:ALA:HB3	1:A:435:PRO:HD3	1.84	0.59
6:C:2026:HOH:O	1:D:72:HIS:HD2	1.85	0.59
1:A:48:LEU:HD11	1:A:114:PHE:HE2	1.67	0.59
1:A:69:TYR:O	1:A:73:LEU:HG	2.03	0.58
1:D:480:LYS:HA	1:D:480:LYS:HE2	1.84	0.58
1:C:397:THR:OG1	1:C:410:LYS:HD3	2.04	0.58
1:B:2:SER:C	1:B:3:LYS:HG2	2.24	0.58
1:A:302:LYS:H	1:A:318:ASN:ND2	2.01	0.58
1:C:189:ARG:NH1	6:C:2102:HOH:O	2.35	0.58
1:C:72:HIS:HD2	6:C:2037:HOH:O	1.87	0.57
1:A:8:VAL:CG2	1:A:153:ALA:HB2	2.34	0.57
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.40	0.57
1:C:403:ILE:HD11	1:D:102:ALA:HB2	1.86	0.57
1:B:341:GLU:OE2	1:B:359:HIS:HE1	1.87	0.57
1:D:29:LYS:HE3	1:D:350:PHE:CD1	2.40	0.57
1:B:316:ARG:HB3	6:B:2203:HOH:O	2.04	0.57
1:D:216:LYS:HE3	1:D:248[A]:GLU:HB2	1.87	0.56
1:D:136:VAL:CG2	1:D:147:VAL:HG13	2.35	0.56
1:A:302:LYS:H	1:A:318:ASN:HD21	1.54	0.56
1:C:31:VAL:N	1:C:119:GLY:O	2.37	0.55
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.42	0.55
1:D:52:CYS:HB3	6:D:2041:HOH:O	2.05	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:266:LYS:N	1:A:266:LYS:HD2	2.21	0.55
1:B:234:ILE:O	1:B:238:VAL:HG12	2.06	0.55
1:A:478:TYR:CE1	1:A:483:LYS:HB2	2.42	0.55
1:D:331:ARG:NH1	1:D:331:ARG:HG3	2.14	0.55
1:C:318:ASN:H	1:C:318:ASN:HD22	1.54	0.55
1:D:237:GLU:HB3	1:D:430:LEU:HD23	1.89	0.54
1:B:2:SER:O	1:B:3:LYS:CG	2.46	0.54
1:A:199:ILE:HD12	4:A:1491:CL:CL	2.45	0.54
1:C:157:LEU:HD13	1:C:345:LEU:CD2	2.38	0.53
1:D:14:SER:HA	3:D:1000:WPF:HAS	1.89	0.53
1:A:299:VAL:HG23	1:A:301:VAL:HG23	1.90	0.53
1:B:335:THR:HB	1:B:336:PRO:HD3	1.90	0.53
1:B:21:TRP:CD1	3:B:1000:WPF:HAX3	2.43	0.53
1:A:400:MET:HB3	6:B:2024:HOH:O	2.08	0.53
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.73	0.53
1:A:289:PRO:HG3	1:A:330:ASP:HB2	1.90	0.53
1:A:68:GLN:NE2	6:A:2057:HOH:O	2.42	0.52
1:C:176:ILE:HB	1:C:180:GLU:HB2	1.90	0.52
1:B:95:LEU:HD22	1:B:210:TYR:CZ	2.44	0.52
1:D:300:GLY:HA2	6:D:2079:HOH:O	2.10	0.52
1:B:400:MET:HG3	1:B:401:HIS:N	2.25	0.52
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.45	0.52
1:B:2:SER:C	1:B:3:LYS:CG	2.78	0.52
1:A:403:ILE:CD1	1:B:62:LEU:HD13	2.40	0.52
1:C:60:LYS:HD2	1:C:60:LYS:C	2.29	0.52
1:B:222:ARG:O	1:B:252:ASN:HA	2.10	0.51
1:B:186:GLU:HB2	1:B:187:PRO:CD	2.41	0.51
1:D:18:GLU:OE1	3:D:1000:WPF:NAV	2.44	0.51
1:B:174:HIS:HE1	6:B:2101:HOH:O	1.93	0.51
1:A:92:TRP:CB	1:A:187:PRO:HG3	2.41	0.51
1:C:76:SER:HB2	1:C:81:TRP:HB2	1.92	0.51
1:A:8:VAL:HG23	1:A:153:ALA:HB2	1.92	0.51
1:B:219:LEU:HD23	1:B:219:LEU:C	2.31	0.51
1:C:113:MET:HG3	3:C:1000:WPF:HAB	1.93	0.51
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE1	2.36	0.50
1:C:110:TYR:CZ	3:C:1000:WPF:HAJ	2.47	0.50
1:A:48:LEU:HD11	1:A:114:PHE:CE2	2.46	0.50
1:C:302:LYS:H	1:C:318:ASN:HD21	1.58	0.50
1:C:171:GLY:HA3	1:C:258:VAL:O	2.11	0.50
1:D:318:ASN:N	1:D:318:ASN:HD22	2.04	0.50
1:C:110:TYR:CE1	3:C:1000:WPF:HAJ	2.46	0.50
1:A:75:GLU:HG2	1:A:404:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:160:THR:OG1	1:C:328:ILE:HD12	2.11	0.50
1:D:95:LEU:HD22	1:D:210:TYR:CZ	2.46	0.50
1:A:221:TYR:CE2	1:A:223:ASN:HB2	2.47	0.50
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.95	0.50
1:B:92:TRP:CZ2	1:B:96:ILE:HD11	2.47	0.50
1:D:261:ASN:ND2	1:D:277:ASP:OD1	2.44	0.49
1:A:14:SER:HA	3:A:1000:WPF:HAS	1.94	0.49
1:D:395:SER:O	1:D:396:PHE:HB3	2.12	0.49
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.95	0.49
1:A:446:ARG:CG	6:A:2339:HOH:O	2.59	0.49
1:A:485:GLU:OE2	1:A:486:LYS:HE2	2.13	0.49
1:B:114:PHE:CE1	1:B:120:LEU:HG	2.47	0.49
1:C:48:LEU:HD11	1:C:114:PHE:HE2	1.78	0.49
1:B:14:SER:HA	3:B:1000:WPF:HAS	1.94	0.49
1:D:29:LYS:HE3	1:D:350:PHE:HD1	1.77	0.48
1:B:232:GLU:O	1:B:236:GLU:HG3	2.12	0.48
1:C:268:VAL:O	1:C:275:THR:HA	2.14	0.48
1:A:421:ASP:O	1:A:450:LYS:HE3	2.12	0.48
1:A:446:ARG:HG3	6:A:2339:HOH:O	2.14	0.48
1:C:438:ILE:O	1:C:441:VAL:HB	2.14	0.48
1:A:329:THR:O	1:A:331[A]:ARG:HD2	2.13	0.48
1:D:52:CYS:CB	6:D:2041:HOH:O	2.59	0.47
1:B:18:GLU:OE1	3:B:1000:WPF:NAV	2.48	0.47
1:A:189:ARG:HA	1:A:212:PRO:HD2	1.95	0.47
1:D:160:THR:OG1	1:D:328:ILE:HD12	2.13	0.47
1:A:225:LEU:H	1:A:228:ARG:HH21	1.63	0.47
1:D:104:LEU:HG	1:D:108:LYS:HE3	1.96	0.47
1:C:38:THR:HG23	1:C:124:LEU:HD13	1.96	0.47
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.78	0.47
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.95	0.47
1:B:331:ARG:HG3	6:B:2207:HOH:O	2.14	0.47
1:D:254:ASN:ND2	1:D:271:GLU:OE2	2.47	0.47
1:B:3:LYS:HE3	1:B:149:GLU:OE1	2.15	0.46
1:D:455:TYR:CE2	1:D:472:ARG:HB2	2.50	0.46
1:B:389:VAL:HB	1:B:478:TYR:HB2	1.97	0.46
1:D:20:GLY:HA2	1:D:31:VAL:HG11	1.98	0.46
1:A:332:LEU:HD13	1:A:337:VAL:HG21	1.98	0.46
1:C:299:VAL:CG2	1:C:301:VAL:HG23	2.42	0.46
1:A:112:GLY:HA3	6:A:2097:HOH:O	2.16	0.46
1:B:222:ARG:NH1	6:B:2140:HOH:O	2.48	0.46
1:C:95:LEU:HD22	1:C:210:TYR:CZ	2.50	0.46
1:D:75:GLU:HB3	1:D:404:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:114:PHE:CE1	1:C:120:LEU:HG	2.51	0.46
1:D:411:PHE:CD1	1:D:431:GLY:HA3	2.51	0.46
1:A:403:ILE:HD12	1:B:62:LEU:HD13	1.98	0.46
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.98	0.46
1:A:52[A]:CYS:HB2	1:A:57:CYS:SG	2.56	0.45
1:A:176:ILE:HB	1:A:180:GLU:HB2	1.98	0.45
1:C:335:THR:HB	1:C:336:PRO:HD3	1.98	0.45
1:A:130:GLU:HB2	1:A:136:VAL:CG2	2.47	0.45
1:C:29:LYS:HA	1:C:29:LYS:HD3	1.71	0.45
1:B:299:VAL:HG23	1:B:301:VAL:HG23	1.99	0.45
1:A:302:LYS:NZ	6:A:2252:HOH:O	2.38	0.45
1:C:113:MET:CB	3:C:1000:WPF:HAB	2.47	0.45
1:A:34:VAL:HA	1:A:123:PHE:O	2.17	0.45
1:C:89:LYS:HE2	6:D:2058:HOH:O	2.16	0.45
1:D:222:ARG:HH12	1:D:254:ASN:ND2	2.15	0.45
1:A:160:THR:OG1	1:A:328:ILE:HD12	2.16	0.45
1:B:154:ASP:O	1:B:321:ASN:HB2	2.17	0.45
1:A:45:TYR:CG	1:A:179:ASN:HB3	2.52	0.45
1:D:474:PRO:HG2	1:D:477:TYR:CE1	2.52	0.45
1:D:222:ARG:NH1	1:D:254:ASN:ND2	2.65	0.44
1:A:109:SER:O	1:A:113:MET:HG3	2.17	0.44
1:A:351:GLY:O	1:A:353:LYS:HG3	2.17	0.44
1:B:130:GLU:OE2	1:B:150:ARG:NH1	2.45	0.44
1:D:446:ARG:NH1	6:D:2314:HOH:O	2.50	0.44
1:B:165:GLN:HB2	1:B:288:ILE:HG23	2.00	0.44
1:B:52:CYS:HB3	6:B:2016:HOH:O	2.17	0.44
1:D:41:GLY:HA2	1:D:183:TYR:CZ	2.53	0.44
1:D:191:VAL:CG1	1:D:217:VAL:HG22	2.47	0.44
1:B:161:GLY:HA2	1:B:327:ASP:HB2	2.00	0.44
1:C:104:LEU:HG	1:C:108:LYS:HE3	1.99	0.44
1:A:114:PHE:CG	1:A:122:PHE:HB2	2.52	0.44
1:B:48:LEU:HD11	1:B:114:PHE:HE2	1.82	0.44
1:C:447:LEU:HD23	1:C:447:LEU:HA	1.78	0.44
1:B:152:GLN:HG2	1:B:152:GLN:H	1.59	0.44
1:D:221:TYR:CZ	1:D:223:ASN:HB2	2.52	0.44
1:A:83:PHE:HB3	1:B:88:VAL:HG22	2.00	0.44
2:B:998:FAD:H9	2:B:998:FAD:H1'1	1.76	0.44
1:A:250:MET:CE	1:A:253:GLU:HG3	2.48	0.44
1:B:48:LEU:HD11	1:B:114:PHE:CE2	2.53	0.44
1:A:13:GLY:HA2	1:A:50:GLY:HA3	1.99	0.44
1:A:396:PHE:CD1	1:A:396:PHE:N	2.86	0.43
1:A:132:LYS:HB2	6:A:2110:HOH:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:331:ARG:CG	1:D:331:ARG:NH1	2.69	0.43
1:C:15:GLY:HA3	1:C:325:ILE:HD12	2.01	0.43
1:C:486:LYS:HD2	1:C:486:LYS:HA	1.82	0.43
1:B:304:THR:HB	1:B:305:PRO:HD2	2.00	0.43
1:B:392:TYR:O	1:B:414:LYS:HA	2.19	0.43
1:B:478:TYR:CE1	1:B:483:LYS:HB2	2.54	0.43
1:A:351:GLY:O	1:A:352:ASN:C	2.57	0.43
1:C:80:GLY:HA2	1:D:94:LYS:HG2	2.00	0.43
1:C:392:TYR:CD2	1:C:392:TYR:N	2.86	0.43
1:A:429:LEU:HD21	1:A:468:LEU:HD21	2.00	0.43
1:C:75:GLU:HB3	1:C:404:SER:HB2	2.00	0.43
1:B:144:LYS:O	1:B:144:LYS:HG2	2.18	0.43
1:D:302:LYS:H	1:D:318:ASN:ND2	2.16	0.43
1:C:231:ASP:HB3	1:C:234:ILE:HB	2.01	0.43
1:A:92:TRP:HB3	1:A:187:PRO:HG3	2.00	0.43
1:A:3:LYS:HB2	1:A:5:PHE:CE2	2.54	0.43
1:C:359:HIS:HB2	6:C:2210:HOH:O	2.19	0.43
1:D:292:ASN:HD22	1:D:292:ASN:HA	1.65	0.43
1:B:114:PHE:CD1	1:B:120:LEU:HG	2.54	0.42
1:D:474:PRO:HG2	1:D:477:TYR:CZ	2.54	0.42
1:B:160:THR:OG1	1:B:328:ILE:HD12	2.19	0.42
1:A:18:GLU:OE1	3:A:1000:WPF:NAV	2.52	0.42
1:C:48:LEU:HD11	1:C:114:PHE:CE2	2.54	0.42
1:A:455:TYR:CZ	1:A:472:ARG:HD2	2.54	0.42
1:D:8:VAL:CG2	1:D:153:ALA:HB2	2.49	0.42
1:A:162:SER:HB3	1:A:327:ASP:HB3	2.00	0.42
1:C:465:ALA:HB1	1:D:439:GLN:HB3	2.02	0.42
1:D:40:HIS:H	1:D:107:ASN:ND2	2.18	0.42
1:B:268:VAL:O	1:B:275:THR:HA	2.20	0.42
1:C:129:LEU:HD11	1:C:156:ILE:HG21	2.00	0.42
1:C:311:VAL:HB	1:C:315:SER:HA	2.02	0.42
1:A:89:LYS:HG2	1:A:90:ALA:N	2.34	0.42
1:C:455:TYR:CD2	1:C:472:ARG:HB3	2.55	0.42
1:D:99:LYS:C	1:D:99:LYS:HD2	2.39	0.42
1:A:248:GLU:HG2	6:A:2178:HOH:O	2.20	0.42
1:C:370:PRO:HG2	1:C:430:LEU:HD11	2.01	0.42
1:C:468:LEU:HA	1:C:468:LEU:HD23	1.85	0.42
1:B:34:VAL:HA	1:B:123:PHE:O	2.20	0.42
1:A:446:ARG:HD2	6:A:2339:HOH:O	2.19	0.42
1:A:395:SER:HA	1:A:411:PHE:O	2.18	0.42
1:C:38:THR:HG22	1:C:122:PHE:CE2	2.54	0.42
1:B:45:TYR:CG	1:B:179:ASN:HB3	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:336:PRO:HG3	1:D:461:HIS:HB2	2.02	0.41
1:C:466:GLU:HA	1:D:439:GLN:OE1	2.19	0.41
1:B:13:GLY:HA2	1:B:50:GLY:HA3	2.01	0.41
1:A:95:LEU:HD22	1:A:210:TYR:CZ	2.54	0.41
1:B:463:THR:O	1:B:466:GLU:HG2	2.20	0.41
1:C:184:LEU:HA	1:C:185:PRO:HD3	1.99	0.41
1:C:41:GLY:HA2	1:C:183:TYR:CZ	2.55	0.41
1:A:99:LYS:C	1:A:99:LYS:HD2	2.41	0.41
1:C:402:ASN:O	6:C:2233:HOH:O	2.22	0.41
1:C:113:MET:CG	3:C:1000:WPF:HAB	2.49	0.41
1:A:92:TRP:HB2	1:A:187:PRO:HG3	2.02	0.41
1:B:152:GLN:HB3	6:B:2092:HOH:O	2.21	0.41
1:A:20:GLY:HA2	1:A:31:VAL:HG11	2.03	0.41
1:C:40:HIS:HB3	1:C:54:ASN:OD1	2.19	0.41
1:C:69:TYR:O	1:C:73:LEU:HG	2.21	0.41
1:C:306:LYS:HB3	1:C:330:ASP:OD2	2.20	0.41
1:A:371:PRO:HD3	6:A:2057:HOH:O	2.21	0.41
1:B:130:GLU:CD	1:B:150:ARG:HH22	2.24	0.41
1:C:130:GLU:OE1	1:C:134:VAL:HG11	2.21	0.41
1:C:113:MET:HB2	3:C:1000:WPF:HAB	2.03	0.41
1:C:60:LYS:HD2	1:C:61:LYS:N	2.36	0.41
1:C:69:TYR:HB2	1:D:81:TRP:NE1	2.35	0.41
1:B:240:LYS:HD2	6:B:2045:HOH:O	2.20	0.41
1:C:8:VAL:CG2	1:C:153:ALA:HB2	2.50	0.41
1:D:223:ASN:ND2	6:D:2167:HOH:O	2.35	0.41
1:B:232:GLU:HA	1:B:235:ARG:HD3	2.03	0.40
1:B:163:TRP:CG	1:B:164:PRO:HD2	2.56	0.40
1:C:443:VAL:O	1:C:446:ARG:HB3	2.22	0.40
1:B:289:PRO:HG3	1:B:330:ASP:HB2	2.03	0.40
1:C:325:ILE:HD13	1:C:342:GLY:HA2	2.03	0.40
1:C:13:GLY:HA2	1:C:50:GLY:CA	2.52	0.40
1:B:390:ALA:HB1	1:B:474:PRO:HB3	2.03	0.40
1:D:304:THR:HB	1:D:305:PRO:CD	2.50	0.40
1:A:437:ILE:HG12	1:A:465:ALA:HB2	2.03	0.40
1:C:267:HIS:CE1	1:C:275:THR:HB	2.57	0.40
1:B:157:LEU:HD21	1:B:325:ILE:CD1	2.52	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	490/495 (99%)	472 (96%)	16 (3%)	2 (0%)	43	29
1	B	487/495 (98%)	468 (96%)	16 (3%)	3 (1%)	33	19
1	C	488/495 (99%)	471 (96%)	15 (3%)	2 (0%)	43	29
1	D	491/495 (99%)	475 (97%)	13 (3%)	3 (1%)	33	19
All	All	1956/1980 (99%)	1886 (96%)	60 (3%)	10 (0%)	38	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	LYS
1	B	3	LYS
1	B	45	TYR
1	D	480	LYS
1	A	480	LYS
1	D	396	PHE
1	C	45	TYR
1	D	55	VAL
1	A	55	VAL
1	B	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	405/407 (100%)	381 (94%)	24 (6%)	28	14
1	B	399/407 (98%)	382 (96%)	17 (4%)	40	26
1	C	403/407 (99%)	382 (95%)	21 (5%)	32	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	405/407 (100%)	382 (94%)	23 (6%)	29	15
All	All	1612/1628 (99%)	1527 (95%)	85 (5%)	33	18

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52[A]	CYS
1	A	52[B]	CYS
1	A	57	CYS
1	A	60	LYS
1	A	94	LYS
1	A	99	LYS
1	A	109	SER
1	A	129	LEU
1	A	132	LYS
1	A	224	ASN
1	A	228	ARG
1	A	238	VAL
1	A	306	LYS
1	A	318	ASN
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	332	LEU
1	A	335	THR
1	A	385	GLU
1	A	387	GLU
1	A	400	MET
1	A	410	LYS
1	A	467	GLU
1	A	480	LYS
1	B	2	SER
1	B	30	ARG
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	113	MET
1	B	144	LYS
1	B	150	ARG
1	B	152	GLN
1	B	213	PRO
1	B	260	LEU
1	B	306	LYS

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Mol	Chain	Res	Type
1	B	321	ASN
1	B	355	ARG
1	B	407	LYS
1	B	480	LYS
1	B	485	GLU
1	C	3	LYS
1	C	30	ARG
1	C	57	CYS
1	C	60	LYS
1	C	93	LYS
1	C	94	LYS
1	C	99	LYS
1	C	113	MET
1	C	128	SER
1	C	129	LEU
1	C	132	LYS
1	C	136	VAL
1	C	139	GLU
1	C	152	GLN
1	C	228	ARG
1	C	259	SER
1	C	260	LEU
1	C	262	THR
1	C	306	LYS
1	C	318	ASN
1	C	486	LYS
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	99	LYS
1	D	149	GLU
1	D	186	GLU
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	231	ASP
1	D	266	LYS
1	D	277	ASP
1	D	290	ARG
1	D	292	ASN
1	D	306	LYS
1	D	318	ASN
1	D	321	ASN

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Mol	Chain	Res	Type
1	D	331	ARG
1	D	353	LYS
1	D	400	MET
1	D	480	LYS
1	D	482	GLU
1	D	485	GLU
1	D	487	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	152	GLN
1	A	318	ASN
1	B	72	HIS
1	B	107	ASN
1	B	174	HIS
1	B	310	GLN
1	B	359	HIS
1	C	72	HIS
1	C	107	ASN
1	C	152	GLN
1	C	310	GLN
1	C	318	ASN
1	D	72	HIS
1	D	107	ASN
1	D	152	GLN
1	D	223	ASN
1	D	292	ASN
1	D	295	GLN
1	D	318	ASN
1	D	321	ASN
1	D	359	HIS

### 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 18 ligands modelled in this entry, 10 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	WPF	A	1000	-	27,27,27	1.90	6 (22%)	38,38,38	1.64	7 (18%)
2	FAD	A	998	-	58,58,58	1.30	6 (10%)	85,89,89	1.83	16 (18%)
3	WPF	B	1000	-	27,27,27	2.11	6 (22%)	38,38,38	1.84	8 (21%)
2	FAD	B	998	-	58,58,58	1.13	4 (6%)	85,89,89	2.09	16 (18%)
3	WPF	C	1000	-	27,27,27	2.32	8 (29%)	38,38,38	1.75	10 (26%)
2	FAD	C	998	-	58,58,58	1.09	4 (6%)	85,89,89	2.29	21 (24%)
3	WPF	D	1000	-	27,27,27	2.05	7 (25%)	38,38,38	1.51	5 (13%)
2	FAD	D	998	-	58,58,58	0.98	3 (5%)	85,89,89	1.83	19 (22%)

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	WPF	A	1000	-	-	0/10/26/26	0/1/3/3
2	FAD	A	998	-	-	0/34/50/50	0/1/6/6
3	WPF	B	1000	-	-	0/10/26/26	0/1/3/3
2	FAD	B	998	-	-	0/34/50/50	0/1/6/6
3	WPF	C	1000	-	-	0/10/26/26	0/1/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	998	-	-	0/34/50/50	0/1/6/6
3	WPF	D	1000	-	-	0/10/26/26	0/1/3/3
2	FAD	D	998	-	-	0/34/50/50	0/1/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	WPF	CAW-NAV	6.67	1.41	1.29
3	C	1000	WPF	CAW-NAV	6.61	1.41	1.29
3	D	1000	WPF	CAW-NAV	6.55	1.41	1.29
3	A	1000	WPF	CAW-NAV	6.35	1.40	1.29
3	C	1000	WPF	CAK-CAL	5.26	1.57	1.52
3	B	1000	WPF	CAW-NAM	4.84	1.43	1.35
3	A	1000	WPF	CAX-CAW	4.02	1.56	1.49
2	B	998	FAD	C2A-N3A	3.93	1.39	1.32
3	D	1000	WPF	CAW-NAM	3.90	1.41	1.35
3	C	1000	WPF	CAW-NAM	3.87	1.41	1.35
3	D	1000	WPF	CAK-CAL	3.86	1.56	1.52
2	A	998	FAD	C5X-N5	3.83	1.41	1.35
2	C	998	FAD	C2A-N3A	3.50	1.39	1.32
3	C	1000	WPF	CAF-CAL	3.37	1.56	1.52
3	B	1000	WPF	CAK-CAL	3.32	1.55	1.52
3	D	1000	WPF	CAN-NAM	3.20	1.51	1.46
3	B	1000	WPF	CAL-NAM	3.19	1.50	1.48
2	A	998	FAD	C1'-C2'	-3.10	1.48	1.51
2	B	998	FAD	C2A-N1A	3.06	1.39	1.33
3	B	1000	WPF	CAX-CAW	2.91	1.54	1.49
3	C	1000	WPF	CAN-NAM	2.88	1.51	1.46
3	D	1000	WPF	CAX-CAW	2.87	1.54	1.49
3	C	1000	WPF	CAX-CAW	2.81	1.54	1.49
3	C	1000	WPF	CAL-NAM	2.74	1.49	1.48
3	A	1000	WPF	CAN-NAM	2.65	1.50	1.46
2	D	998	FAD	P-O3P	-2.63	1.55	1.59
3	A	1000	WPF	CAK-CAL	2.57	1.54	1.52
3	C	1000	WPF	CAJ-CAI	2.52	1.42	1.38
3	A	1000	WPF	CAJ-CAI	2.48	1.42	1.38
2	A	998	FAD	C1'-N10	2.47	1.51	1.48
2	C	998	FAD	C5X-N5	2.43	1.39	1.35
2	B	998	FAD	C9A-C5X	-2.34	1.37	1.42
2	C	998	FAD	C4-C4X	-2.28	1.37	1.41
2	C	998	FAD	C2A-N1A	2.24	1.38	1.33
3	A	1000	WPF	CAW-NAM	2.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	WPF	CAF-CAL	2.19	1.55	1.52
3	B	1000	WPF	CAS-CAI	2.18	1.42	1.38
2	A	998	FAD	O3B-C3B	2.17	1.48	1.43
2	D	998	FAD	C5X-N5	2.10	1.38	1.35
3	D	1000	WPF	CAE-CAF	2.09	1.42	1.39
2	A	998	FAD	C8A-N9A	2.08	1.39	1.36
2	A	998	FAD	C4A-N3A	2.05	1.38	1.35
2	B	998	FAD	C1'-C2'	-2.04	1.49	1.51
2	D	998	FAD	C2A-N3A	2.03	1.36	1.32

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	998	FAD	N3A-C2A-N1A	-11.77	118.87	128.71
2	B	998	FAD	N3A-C2A-N1A	-9.74	120.56	128.71
2	A	998	FAD	N3A-C2A-N1A	-9.10	121.11	128.71
2	B	998	FAD	O4B-C1B-N9A	-7.98	101.02	108.44
2	D	998	FAD	N3A-C2A-N1A	-7.64	122.32	128.71
3	A	1000	WPF	CAF-CAL-NAM	-5.96	102.48	111.54
2	B	998	FAD	C4X-N5-C5X	5.60	122.98	116.69
3	B	1000	WPF	CAF-CAL-NAM	-5.50	103.19	111.54
2	C	998	FAD	C2-N1-C10	5.16	120.18	114.98
2	C	998	FAD	C4X-N5-C5X	5.14	122.46	116.69
2	D	998	FAD	C4X-N5-C5X	4.94	122.24	116.69
2	B	998	FAD	C2-N1-C10	4.86	119.88	114.98
2	A	998	FAD	C2-N1-C10	4.76	119.77	114.98
2	A	998	FAD	C2A-N1A-C6A	4.72	127.29	118.77
2	C	998	FAD	C1'-N10-C9A	4.63	123.37	118.87
2	C	998	FAD	C4X-C10-N1	-4.52	118.22	122.73
3	B	1000	WPF	CAX-CAW-NAM	4.50	123.23	117.85
2	D	998	FAD	O4B-C1B-N9A	-4.33	104.41	108.44
2	C	998	FAD	C5X-C9A-N10	4.10	120.84	116.80
3	C	1000	WPF	CAU-NAV-CAW	4.09	123.54	118.38
3	B	1000	WPF	CAU-NAV-CAW	4.04	123.48	118.38
3	D	1000	WPF	CAF-CAL-NAM	-3.96	105.53	111.54
3	C	1000	WPF	CAS-CAI-CAJ	-3.90	116.14	121.54
2	C	998	FAD	N3A-C4A-N9A	3.88	132.44	125.43
2	A	998	FAD	C4X-N5-C5X	3.86	121.03	116.69
3	D	1000	WPF	CAU-NAV-CAW	3.84	123.23	118.38
2	D	998	FAD	C2'-C1'-N10	3.73	117.40	112.45
2	D	998	FAD	C2-N1-C10	3.64	118.64	114.98
2	C	998	FAD	C9A-N10-C10	-3.54	118.29	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	998	FAD	C4A-C5A-N7A	-3.52	106.51	109.52
2	B	998	FAD	N3A-C4A-N9A	3.51	131.76	125.43
2	C	998	FAD	C4B-O4B-C1B	-3.48	105.97	109.75
3	C	1000	WPF	CAI-CAJ-CAK	3.38	123.88	120.08
2	B	998	FAD	C4-C4X-C10	3.38	122.41	116.95
2	D	998	FAD	C5X-C9A-N10	3.28	120.03	116.80
3	D	1000	WPF	CAK-CAU-NAV	-3.25	118.83	122.22
2	C	998	FAD	C9A-C5X-N5	-3.25	117.39	122.37
2	D	998	FAD	C4'-C3'-C2'	-3.25	105.90	113.25
2	A	998	FAD	C4X-C10-N1	-3.22	119.51	122.73
3	B	1000	WPF	CAT-CAU-CAK	3.21	122.43	119.56
2	C	998	FAD	C4-C4X-C10	3.20	122.11	116.95
2	D	998	FAD	C4B-O4B-C1B	-3.09	106.39	109.75
2	B	998	FAD	C5X-C9A-N10	3.07	119.83	116.80
3	B	1000	WPF	CAX-CAW-NAV	-3.07	115.96	119.68
2	D	998	FAD	N3A-C4A-N9A	3.03	130.90	125.43
3	C	1000	WPF	CAO-CAN-NAM	-3.00	109.27	113.44
2	B	998	FAD	C4X-C10-N1	-2.94	119.79	122.73
2	B	998	FAD	C4B-O4B-C1B	-2.93	106.56	109.75
3	B	1000	WPF	CAK-CAU-NAV	-2.84	119.27	122.22
3	C	1000	WPF	CAF-CAL-NAM	-2.83	107.23	111.54
2	C	998	FAD	O3'-C3'-C2'	-2.79	101.69	108.74
2	A	998	FAD	O2'-C2'-C3'	2.73	115.86	109.05
2	B	998	FAD	C4A-C5A-N7A	-2.71	107.20	109.52
2	B	998	FAD	O4B-C1B-C2B	-2.70	102.63	106.77
3	A	1000	WPF	CAN-NAM-CAL	2.69	121.83	117.87
3	C	1000	WPF	CAK-CAU-NAV	-2.68	119.43	122.22
2	B	998	FAD	C2'-C1'-N10	-2.66	108.93	112.45
2	C	998	FAD	N7A-C8A-N9A	-2.62	106.95	114.36
2	A	998	FAD	C4-N3-C2	-2.59	120.08	125.39
2	D	998	FAD	C8A-N9A-C4A	2.58	108.87	106.90
3	C	1000	WPF	CAX-CAW-NAM	2.56	120.91	117.85
2	C	998	FAD	C8A-N9A-C4A	2.55	108.85	106.90
3	A	1000	WPF	CAO-CAP-NAQ	-2.52	106.98	113.59
2	B	998	FAD	C9A-N10-C10	-2.51	119.30	121.77
2	A	998	FAD	O4'-C4'-C5'	-2.51	104.97	110.12
2	D	998	FAD	N7A-C8A-N9A	-2.49	107.31	114.36
2	C	998	FAD	C4-N3-C2	-2.48	120.30	125.39
2	C	998	FAD	O2A-PA-O3P	2.47	116.85	105.14
2	D	998	FAD	C4-C4X-C10	2.43	120.88	116.95
2	B	998	FAD	C9A-C5X-N5	-2.43	118.64	122.37
2	A	998	FAD	C4-C4X-C10	2.43	120.87	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1000	WPF	CAX-CAW-NAM	2.42	120.74	117.85
2	C	998	FAD	O4B-C1B-N9A	-2.41	106.20	108.44
3	A	1000	WPF	CAU-NAV-CAW	2.37	121.38	118.38
2	C	998	FAD	O5'-P-O1P	-2.37	100.08	109.37
3	C	1000	WPF	CAK-CAL-NAM	2.35	114.11	110.65
2	D	998	FAD	C9A-N10-C10	-2.35	119.46	121.77
2	D	998	FAD	C9A-C5X-N5	-2.34	118.78	122.37
2	A	998	FAD	C1'-C2'-C3'	-2.34	103.14	109.82
3	C	1000	WPF	CAJ-CAI-CL1	2.33	122.03	119.14
3	A	1000	WPF	CAT-CAU-CAK	2.30	121.61	119.56
2	C	998	FAD	C5B-C4B-C3B	-2.27	106.11	115.21
2	A	998	FAD	O4B-C1B-C2B	-2.25	103.32	106.77
2	A	998	FAD	C4B-O4B-C1B	-2.23	107.33	109.75
3	A	1000	WPF	CAB-CAE-CAF	-2.22	118.85	121.20
3	C	1000	WPF	CAN-NAM-CAL	2.20	121.10	117.87
2	A	998	FAD	N3A-C4A-N9A	2.19	129.39	125.43
2	A	998	FAD	O4B-C1B-N9A	-2.16	106.43	108.44
2	D	998	FAD	C4X-C10-N1	-2.14	120.59	122.73
3	D	1000	WPF	CAT-CAU-CAK	2.14	121.47	119.56
3	B	1000	WPF	CAF-CAL-CAK	-2.11	108.82	112.54
2	A	998	FAD	C5'-C4'-C3'	-2.10	108.10	112.06
2	B	998	FAD	N7A-C8A-N9A	-2.10	108.42	114.36
2	C	998	FAD	C1B-N9A-C4A	-2.09	123.02	126.64
2	D	998	FAD	C8A-N7A-C5A	2.08	110.02	103.58
2	D	998	FAD	C6-C5X-C9A	2.06	121.87	119.02
2	B	998	FAD	C6-C5X-N5	2.04	121.35	118.97
3	B	1000	WPF	CAK-CAL-NAM	2.04	113.65	110.65
2	D	998	FAD	O5B-C5B-C4B	-2.04	101.46	108.94
2	C	998	FAD	C7-C6-C5X	-2.01	117.53	120.91
2	A	998	FAD	O3'-C3'-C2'	2.00	113.79	108.74
3	A	1000	WPF	CAK-CAU-NAV	-2.00	120.14	122.22

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	490/495 (98%)	-0.38	2 (0%) 90 91	9, 19, 33, 46	0
1	B	487/495 (98%)	-0.24	5 (1%) 79 81	13, 24, 41, 53	0
1	C	487/495 (98%)	-0.15	6 (1%) 75 78	12, 24, 45, 57	0
1	D	491/495 (99%)	-0.36	2 (0%) 90 91	10, 20, 33, 47	0
All	All	1955/1980 (98%)	-0.28	15 (0%) 83 85	9, 21, 41, 57	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	ASN	3.6
1	C	352	ASN	3.6
1	C	305	PRO	3.4
1	D	305	PRO	3.2
1	C	306	LYS	3.1
1	B	305	PRO	2.8
1	A	352	ASN	2.7
1	B	353	LYS	2.6
1	C	144	LYS	2.6
1	B	306	LYS	2.4
1	B	2	SER	2.4
1	D	488	PRO	2.3
1	C	152	GLN	2.3
1	A	305	PRO	2.1
1	C	354	PRO	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
3	WPF	C	1000	25/25	0.26	5.51	48,62,66,67	0
3	WPF	B	1000	25/25	0.20	4.14	36,41,54,55	0
3	WPF	D	1000	25/25	0.14	4.08	25,32,43,46	0
3	WPF	A	1000	25/25	0.15	2.62	22,30,47,48	0
5	BR	B	1491	1/1	0.16	1.02	69,69,69,69	0
4	CL	B	1489	1/1	0.10	0.63	17,17,17,17	0
4	CL	A	1489	1/1	0.10	0.39	17,17,17,17	0
2	FAD	D	998	53/53	0.08	-0.03	11,14,18,19	0
2	FAD	B	998	53/53	0.08	-0.37	15,21,27,28	0
4	CL	A	1490	1/1	0.08	-0.38	19,19,19,19	0
5	BR	D	1489	1/1	0.10	-0.56	66,66,66,66	0
2	FAD	C	998	53/53	0.07	-0.71	13,21,27,28	0
4	CL	B	1490	1/1	0.07	-0.78	18,18,18,18	0
2	FAD	A	998	53/53	0.07	-0.83	2,12,16,17	0
4	CL	C	1490	1/1	0.07	-0.98	15,15,15,15	0
4	CL	C	1491	1/1	0.04	-1.29	22,22,22,22	0
5	BR	D	1490	1/1	0.02	-2.48	36,36,36,36	0
4	CL	A	1491	1/1	0.04	-2.68	27,27,27,27	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.