



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 01:47 AM GMT

PDB ID : 2WPE
Title : TRYPANOSOMA BRUCEI TRYPANOTHIONE REDUCTASE IN COM-
PLEX WITH 3,4-DIHYDROQUINAZOLINEINHIBITOR (DDD00073359)
Authors : Alphey, M.S.; Patterson, S.; Fairlamb, A.H.
Deposited on : 2009-08-06
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

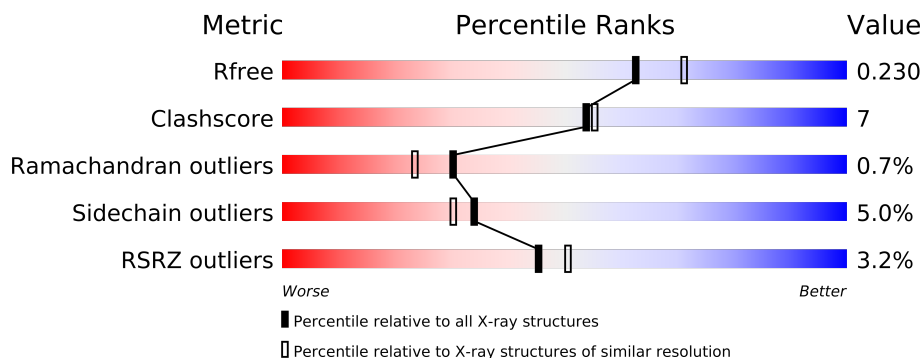
The following versions of software and data (see [references](#)) were used in the production of this report:

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 ≥ 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	WPE	D	1000	-	X
6	MPD	A	1494	-	X
7	MRD	D	1492	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16447 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
			3735	2375	637	703	20			
1	B	486	Total	C	N	O	S	0	2	0
			3704	2358	631	696	19			
1	C	484	Total	C	N	O	S	0	4	0
			3698	2352	628	699	19			
1	D	489	Total	C	N	O	S	0	4	0
			3732	2371	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 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: $C_{27}H_{33}N_9O_{15}P_2$).

Image for chem-comp FAD is not available.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 N-{2-[(4S)-6-CHLORO-2-METHYL-4-PHENYLQUINAZOLIN-3(4H)-YL]ETHYL}FURAN-2-CARBOXAMIDE (three-letter code: WPE) (formula: C₂₂H₂₀ClN₃O₂).

Image for chem-comp WPE is not available.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		
3	B	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		
3	C	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		
3	D	1	Total	C	Cl	N	O	0	0
			28	22	1	3	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total	Cl	0	0
			5	5		
5	A	4	Total	Cl	0	0
			4	4		
5	D	4	Total	Cl	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	5	Total	Cl	0	0
			5	5		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).

Image for chem-comp MPD is not available.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).

Image for chem-comp MRD is not available.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

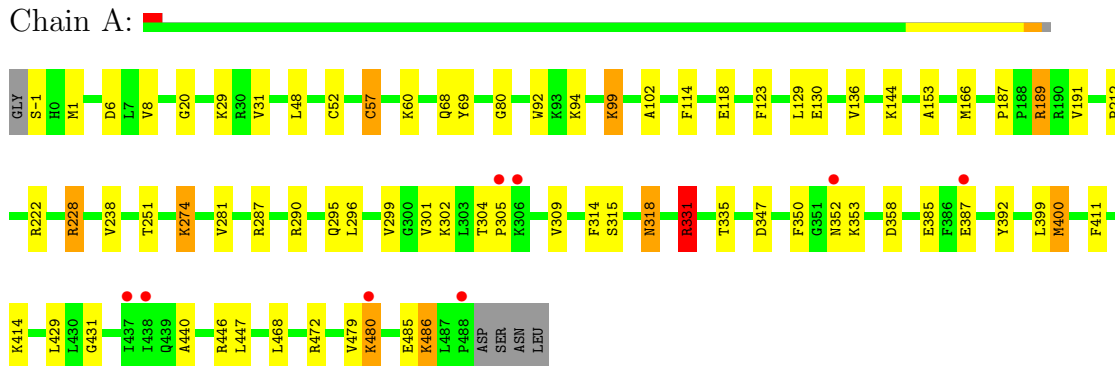
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	365	Total	O	0	0
			365	365		
8	B	265	Total	O	0	0
			265	265		
8	C	265	Total	O	0	0
			265	265		
8	D	321	Total	O	0	0
			321	321		

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.

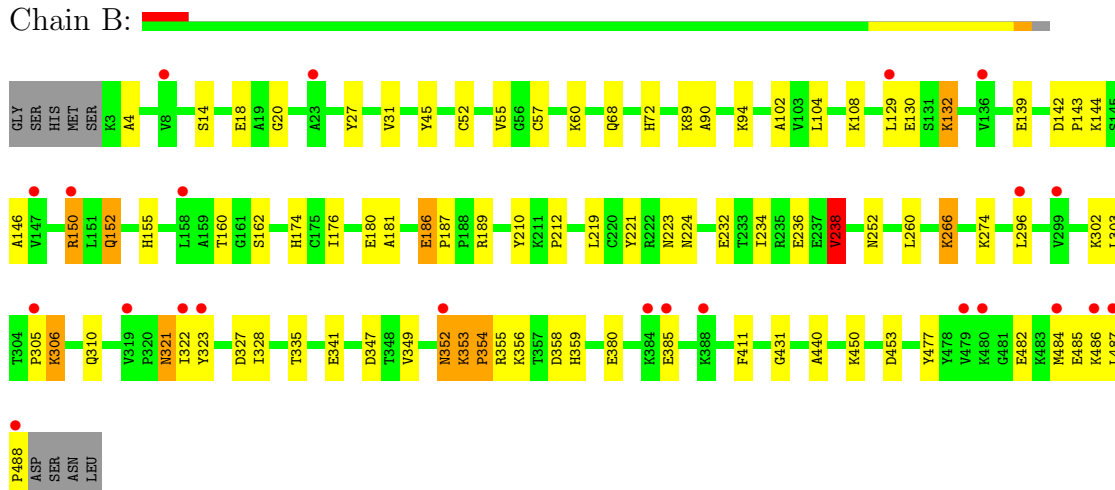
• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain A:



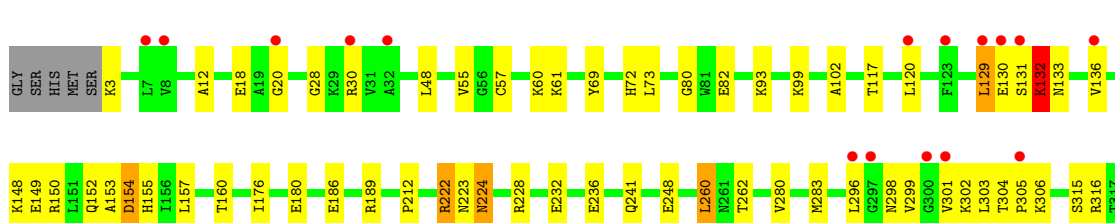
• Molecule 1: TRYPANOTHIONE REDUCTASE

Chain B:



• Molecule 1: TRYPANOTHIONE REDUCTASE

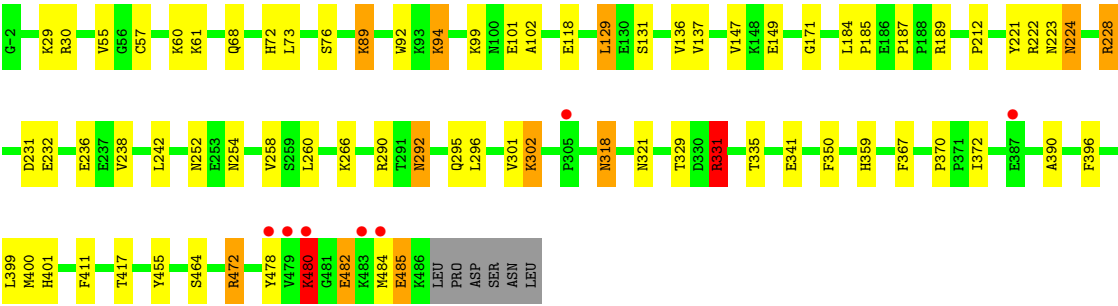
Chain C:





• 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, α , β , γ	100.64Å 63.29Å 169.16Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	45.98 – 2.10 45.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.98-2.10) 99.9 (45.98-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.168 , 0.230 0.168 , 0.230	Depositor DCC
R_{free} test set	6169 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 123374 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16447	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: MPD, CL, NA, MRD, WPE, FAD

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	1.22	8/3820 (0.2%)	1.04	11/5181 (0.2%)
1	B	1.09	4/3787 (0.1%)	0.92	4/5135 (0.1%)
1	C	1.08	1/3787 (0.0%)	0.91	6/5138 (0.1%)
1	D	1.14	1/3822 (0.0%)	0.94	4/5183 (0.1%)
All	All	1.13	14/15216 (0.1%)	0.95	25/20637 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	281	VAL	CB-CG2	7.42	1.68	1.52
1	A	118	GLU	CG-CD	6.82	1.62	1.51
1	A	52	CYS	CB-SG	-6.65	1.71	1.82
1	B	186	GLU	CB-CG	-5.89	1.41	1.52
1	A	123	PHE	CD2-CE2	5.87	1.50	1.39
1	B	380	GLU	CG-CD	5.86	1.60	1.51
1	A	102	ALA	CA-CB	5.83	1.64	1.52
1	A	191	VAL	CB-CG2	5.78	1.65	1.52
1	A	69	TYR	CD1-CE1	5.58	1.47	1.39
1	C	280	VAL	CB-CG2	5.54	1.64	1.52
1	B	238	VAL	CB-CG1	-5.27	1.41	1.52
1	B	181	ALA	CA-CB	5.14	1.63	1.52
1	A	309	VAL	CB-CG1	5.07	1.63	1.52
1	D	118	GLU	CD-OE1	5.03	1.31	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331[A]	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	A	331[B]	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	A	331[A]	ARG	NE-CZ-NH1	10.56	125.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331[B]	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	A	189	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	A	189	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	B	358	ASP	CB-CG-OD1	7.62	125.16	118.30
1	D	260	LEU	CA-CB-CG	7.13	131.70	115.30
1	C	222	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	94	LYS	CD-CE-NZ	-6.45	96.86	111.70
1	C	327	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	488	PRO	N-CA-CB	6.24	110.79	103.30
1	B	266	LYS	CD-CE-NZ	-6.12	97.63	111.70
1	A	6	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	347	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	287	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	30	ARG	CA-CB-CG	-5.73	100.78	113.40
1	D	302	LYS	CD-CE-NZ	-5.64	98.72	111.70
1	C	228	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	B	347	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	327	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	290	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	358	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	283	MET	CG-SD-CE	-5.12	92.01	100.20
1	C	260	LEU	CA-CB-CG	5.03	126.87	115.30

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	3735	0	3751	44	0
1	B	3704	0	3723	52	0
1	C	3698	0	3709	64	0
1	D	3732	0	3737	54	0
2	A	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	28	0	20	1	0
3	B	28	0	20	3	0
3	C	28	0	20	1	0
3	D	28	0	20	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	4	0	0	2	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	4	0	0	0	0
6	A	8	0	14	2	0
7	D	8	0	14	0	0
8	A	365	0	0	11	0
8	B	265	0	0	7	0
8	C	265	0	0	4	0
8	D	321	0	0	12	0
All	All	16447	0	15152	209	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 7.

All (209) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:321:ASN:HB2	8:D:2232:HOH:O	1.41	1.17
1:A:485:GLU:HG2	1:A:486:LYS:HD2	1.20	1.08
1:D:292:ASN:HB2	8:D:2213:HOH:O	1.71	0.91
1:C:130:GLU:HB2	1:C:136:VAL:CG2	2.00	0.90
1:B:352:ASN:C	1:B:352:ASN:HD22	1.74	0.90
1:C:241:GLN:OE1	1:C:370:PRO:HG3	1.72	0.88
1:C:155:HIS:HD1	1:C:323:TYR:HH	1.19	0.87
1:D:318:ASN:H	1:D:318:ASN:HD22	1.18	0.86
1:D:341:GLU:OE2	1:D:359:HIS:HE1	1.64	0.81
1:B:305:PRO:O	1:B:306:LYS:HB2	1.80	0.81
1:B:224:ASN:HD22	1:B:252:ASN:HD21	1.30	0.80
1:C:304:THR:HB	1:C:305:PRO:HD2	1.65	0.78
1:A:485:GLU:HG2	1:A:486:LYS:CD	2.08	0.76
1:C:20:GLY:O	1:C:120:LEU:HD13	1.85	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:370:PRO:HD2	8:D:2261:HOH:O	1.86	0.76
1:C:93:LYS:NZ	1:C:186[B]:GLU:OE2	2.20	0.75
1:A:318:ASN:H	1:A:318:ASN:HD22	1.36	0.74
1:C:155:HIS:HB3	1:C:323:TYR:HE2	1.53	0.73
1:C:301:VAL:HA	1:C:318:ASN:HD21	1.54	0.72
1:D:101[B]:GLU:HG2	8:D:2065:HOH:O	1.90	0.72
1:C:132:LYS:HD2	1:C:321[B]:ASN:OD1	1.91	0.70
1:C:117:THR:O	8:C:2059:HOH:O	2.11	0.69
1:B:274[A]:LYS:HG3	8:B:2156:HOH:O	1.92	0.68
1:D:455:TYR:CE2	1:D:472:ARG:HB2	2.29	0.67
1:A:166:MET:HG3	6:A:1494:MPD:H53	1.79	0.65
1:C:80:GLY:HA2	1:D:94:LYS:HG2	1.79	0.65
1:A:400:MET:HB3	8:A:2051:HOH:O	1.96	0.65
1:B:155:HIS:HB3	1:B:323:TYR:HE2	1.61	0.65
1:B:132:LYS:HZ2	1:B:132:LYS:HB3	1.61	0.65
1:B:234:ILE:O	1:B:238:VAL:HG12	1.97	0.64
8:A:2061:HOH:O	1:B:72:HIS:HD2	1.81	0.63
1:D:189:ARG:HA	1:D:212:PRO:HD2	1.80	0.62
1:A:129:LEU:HD22	1:A:296:LEU:HD23	1.82	0.62
1:B:352:ASN:C	1:B:352:ASN:ND2	2.49	0.62
1:D:318:ASN:ND2	1:D:318:ASN:H	1.94	0.62
1:B:482:GLU:HG3	1:B:484:MET:CE	2.29	0.62
1:B:186:GLU:HB2	1:B:187:PRO:CD	2.29	0.62
1:D:318:ASN:N	1:D:318:ASN:HD22	1.94	0.62
1:B:224:ASN:ND2	1:B:252:ASN:HD21	1.98	0.62
1:D:482:GLU:HG2	1:D:484:MET:CE	2.30	0.61
1:C:133:ASN:ND2	1:C:153:ALA:O	2.22	0.61
1:B:186:GLU:HB2	1:B:187:PRO:HD2	1.83	0.60
1:C:318:ASN:H	1:C:318:ASN:HD22	1.47	0.60
1:D:329:THR:OG1	1:D:331[A]:ARG:NH1	2.35	0.60
1:C:222:ARG:HD2	5:C:1490:CL:CL	2.39	0.60
1:D:390:ALA:HB3	1:D:417:THR:OG1	2.00	0.60
1:D:232:GLU:O	1:D:236:GLU:HG3	2.02	0.60
1:B:341:GLU:OE2	1:B:359:HIS:HE1	1.84	0.59
1:D:331[A]:ARG:HH11	1:D:331[A]:ARG:HB2	1.67	0.58
1:C:485:GLU:HB3	8:C:2259:HOH:O	2.02	0.58
1:C:315:SER:O	1:C:323:TYR:HB3	2.04	0.58
1:A:429:LEU:HD21	1:A:468:LEU:HD21	1.86	0.58
1:B:4:ALA:HA	1:B:152:GLN:HG2	1.85	0.58
1:A:304:THR:HB	1:A:305:PRO:HD2	1.86	0.58
1:C:348:THR:O	1:C:348:THR:HG22	2.04	0.57
1:C:130:GLU:HB2	1:C:136:VAL:HG22	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:148:LYS:O	1:C:149:GLU:HG2	2.05	0.57
1:C:148:LYS:C	1:C:149:GLU:HG2	2.25	0.57
1:D:331[A]:ARG:NH2	8:D:2236:HOH:O	2.34	0.57
1:C:370:PRO:HG2	1:C:430:LEU:HD11	1.85	0.56
1:A:295:GLN:NE2	8:A:2233:HOH:O	2.38	0.56
1:B:353:LYS:O	1:B:354:PRO:C	2.45	0.55
1:A:411:PHE:CD1	1:A:431:GLY:HA3	2.40	0.55
1:C:319:VAL:HG11	1:C:322:ILE:HD12	1.87	0.55
1:C:61:LYS:HE3	1:C:367:PHE:CE1	2.41	0.55
1:B:104:LEU:HG	1:B:108:LYS:HE3	1.87	0.55
1:A:446:ARG:NE	8:A:2330:HOH:O	2.38	0.55
1:A:446:ARG:HB2	8:A:2285:HOH:O	2.07	0.55
1:B:162:SER:HB3	1:B:327:ASP:HB3	1.89	0.55
1:C:296:LEU:HD12	1:C:303:LEU:HD21	1.88	0.55
1:A:29:LYS:HD2	1:A:350:PHE:CD1	2.42	0.54
1:C:93:LYS:HZ1	1:C:186[B]:GLU:CD	2.11	0.54
1:C:132:LYS:HG3	1:C:133:ASN:OD1	2.07	0.54
1:A:228:ARG:NH2	5:A:1493:CL:CL	2.67	0.54
1:D:480:LYS:HA	1:D:480:LYS:HE3	1.89	0.54
1:C:223:ASN:HB3	1:C:224[A]:ASN:OD1	2.07	0.54
1:A:68:GLN:NE2	8:A:2058:HOH:O	2.39	0.53
1:D:29:LYS:HE3	1:D:350:PHE:CD1	2.44	0.53
1:C:403:ILE:HD11	1:D:102:ALA:HB2	1.90	0.53
1:C:73:LEU:CD2	1:D:73:LEU:HD23	2.39	0.53
1:D:72:HIS:HD2	8:D:2053:HOH:O	1.91	0.53
1:C:154:ASP:HB3	1:C:155:HIS:CD2	2.44	0.52
1:D:171:GLY:HA3	1:D:258:VAL:O	2.08	0.52
1:B:18:GLU:OE1	3:B:1000:WPE:NAU	2.42	0.52
1:C:329:THR:OG1	1:C:331:ARG:HD2	2.09	0.51
1:C:131:SER:O	1:C:133:ASN:N	2.44	0.51
1:C:176:ILE:HB	1:C:180:GLU:HB2	1.91	0.51
1:B:219:LEU:HD23	1:B:219:LEU:C	2.31	0.51
1:D:221:TYR:CE2	1:D:223:ASN:HB2	2.46	0.51
1:C:299:VAL:HG23	1:C:301:VAL:HG23	1.92	0.51
1:C:160:THR:OG1	1:C:328:ILE:HD12	2.11	0.51
1:C:130:GLU:HB2	1:C:136:VAL:HG21	1.90	0.50
1:A:301:VAL:HA	1:A:318:ASN:HD21	1.75	0.50
1:C:82:GLU:OE1	1:D:89:LYS:HE3	2.10	0.50
1:D:359:HIS:HD2	8:D:2254:HOH:O	1.95	0.50
1:B:132:LYS:NZ	1:B:321:ASN:OD1	2.44	0.50
1:B:232:GLU:O	1:B:236:GLU:HG3	2.11	0.50
1:C:93:LYS:NZ	1:C:186[B]:GLU:CD	2.65	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:189:ARG:HA	1:B:212:PRO:HD2	1.93	0.50
1:D:136:VAL:HG13	1:D:147:VAL:HG13	1.94	0.50
1:C:189:ARG:HA	1:C:212:PRO:HD2	1.92	0.50
1:C:304:THR:HB	1:C:305:PRO:CD	2.38	0.50
1:B:14:SER:HA	3:B:1000:WPE:HAR	1.94	0.50
1:A:440:ALA:HB3	1:B:440:ALA:HB3	1.93	0.50
1:A:302:LYS:H	1:A:318:ASN:ND2	2.09	0.49
1:C:232:GLU:O	1:C:236:GLU:HG3	2.12	0.49
1:B:296:LEU:HD12	1:B:303:LEU:HD21	1.94	0.49
1:A:20:GLY:HA2	1:A:31:VAL:HG11	1.94	0.49
1:B:305:PRO:O	1:B:306:LYS:CB	2.53	0.49
1:D:61:LYS:HE3	1:D:367:PHE:CE1	2.47	0.49
1:D:321:ASN:CB	8:D:2232:HOH:O	2.23	0.49
1:B:130:GLU:OE1	1:B:150:ARG:NH2	2.45	0.49
1:D:222:ARG:HH12	1:D:254:ASN:ND2	2.10	0.49
1:D:370:PRO:HG2	8:D:2176:HOH:O	2.13	0.49
6:A:1494:MPD:H51	8:A:2134:HOH:O	2.13	0.49
1:B:274[A]:LYS:HG2	8:B:2155:HOH:O	2.14	0.48
1:D:295:GLN:NE2	8:D:2216:HOH:O	2.45	0.48
1:C:302:LYS:H	1:C:318:ASN:ND2	2.11	0.48
1:D:222:ARG:NH1	1:D:254:ASN:ND2	2.62	0.48
1:A:222:ARG:NH2	5:A:1490:CL:CL	2.84	0.48
1:A:302:LYS:H	1:A:318:ASN:HD21	1.62	0.48
1:B:352:ASN:ND2	1:B:352:ASN:O	2.47	0.47
1:C:155:HIS:ND1	1:C:323:TYR:OH	2.27	0.47
1:B:176:ILE:HB	1:B:180:GLU:HB2	1.96	0.47
1:A:130:GLU:HB2	1:A:136:VAL:HG23	1.95	0.47
1:D:301:VAL:HA	1:D:318:ASN:HD21	1.79	0.47
1:C:69:TYR:CD1	1:D:76:SER:HB3	2.50	0.47
1:B:310:GLN:HB3	8:B:2172:HOH:O	2.14	0.47
1:C:155:HIS:HB3	1:C:323:TYR:CE2	2.43	0.47
3:A:1000:WPE:HAM2	3:A:1000:WPE:HAW1	1.69	0.46
1:A:314:PHE:O	1:A:315:SER:HB2	2.16	0.46
1:B:139:GLU:HG3	1:B:146:ALA:HB3	1.97	0.46
1:C:12:ALA:HB1	1:C:48:LEU:HD12	1.96	0.46
1:C:349:VAL:HG12	1:C:350:PHE:CE1	2.51	0.46
1:D:136:VAL:HG12	1:D:137:VAL:N	2.31	0.46
1:D:68:GLN:NE2	8:D:2045:HOH:O	2.48	0.46
1:D:478:TYR:HA	1:D:482:GLU:O	2.15	0.45
1:A:331[A]:ARG:NH2	8:A:2260:HOH:O	2.49	0.45
1:B:52:CYS:HB2	1:B:335:THR:OG1	2.16	0.45
1:C:72:HIS:HD2	8:C:2033:HOH:O	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:302:LYS:H	1:D:318:ASN:ND2	2.14	0.45
1:C:18:GLU:OE1	3:C:1000:WPE:NAU	2.49	0.45
1:A:385:GLU:HB3	8:A:2300:HOH:O	2.17	0.45
1:A:99:LYS:C	1:A:99:LYS:HD2	2.37	0.45
1:B:477:TYR:CD1	1:B:487:LEU:HD13	2.52	0.45
1:C:320:PRO:O	1:C:321[B]:ASN:OD1	2.34	0.45
1:C:372:ILE:HG22	1:C:373:GLY:N	2.32	0.45
1:A:392:TYR:O	1:A:414:LYS:HA	2.17	0.44
1:B:221:TYR:CE2	1:B:223:ASN:HB2	2.51	0.44
3:D:1000:WPE:HAW1	3:D:1000:WPE:HAM2	1.84	0.44
1:B:132:LYS:NZ	1:B:132:LYS:HB3	2.31	0.44
1:B:90:ALA:HB1	1:B:210:TYR:CD1	2.53	0.44
1:A:57:CYS:HB3	2:A:998:FAD:C4	2.47	0.44
1:A:8:VAL:CG2	1:A:153:ALA:HB2	2.48	0.44
1:D:129:LEU:HD22	1:D:296:LEU:HD23	1.99	0.44
1:C:316:ARG:HG2	1:C:323:TYR:CD1	2.53	0.43
1:D:411:PHE:CZ	1:D:464:SER:HB3	2.53	0.43
1:A:304:THR:HB	1:A:305:PRO:CD	2.48	0.43
1:C:102:ALA:HB1	1:D:399:LEU:HD11	2.00	0.43
1:A:318:ASN:H	1:A:318:ASN:ND2	2.11	0.43
1:A:479:VAL:O	1:A:480:LYS:C	2.57	0.43
1:B:411:PHE:CD1	1:B:431:GLY:HA3	2.53	0.43
1:D:184:LEU:HA	1:D:185:PRO:HD3	1.94	0.43
1:B:160:THR:OG1	1:B:328:ILE:HD12	2.18	0.43
1:B:266:LYS:HD2	1:B:266:LYS:N	2.33	0.43
1:C:130:GLU:CB	1:C:136:VAL:CG2	2.86	0.42
1:D:482:GLU:HG2	1:D:484:MET:HE3	2.00	0.42
1:C:358:ASP:OD2	1:C:446:ARG:NH2	2.51	0.42
1:D:92:TRP:HB3	1:D:187:PRO:HD3	2.01	0.42
1:A:399:LEU:HD11	1:B:102:ALA:HB1	1.99	0.42
1:B:450:LYS:NZ	8:B:2239:HOH:O	2.51	0.42
1:C:341:GLU:OE2	1:C:359:HIS:HE1	2.02	0.42
1:D:485:GLU:OE1	1:D:485:GLU:N	2.53	0.42
1:A:446:ARG:NH1	1:B:453:ASP:OD1	2.52	0.42
1:A:80:GLY:HA2	1:B:94:LYS:HG2	2.01	0.42
1:C:157:LEU:HD11	1:C:325:ILE:HG12	2.01	0.42
1:B:20:GLY:HA2	1:B:31:VAL:HG11	2.02	0.42
1:D:238:VAL:HG21	1:D:372:ILE:HD11	2.01	0.42
1:C:331:ARG:N	8:C:2191:HOH:O	2.53	0.41
1:D:136:VAL:CG1	1:D:137:VAL:N	2.82	0.41
1:B:52:CYS:HB3	8:B:2015:HOH:O	2.20	0.41
1:A:68:GLN:HB3	8:A:2059:HOH:O	2.19	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:GLN:NE2	8:B:2022:HOH:O	2.46	0.41
1:C:318:ASN:HD22	1:C:318:ASN:N	2.16	0.41
1:B:27:TYR:OH	1:B:353:LYS:HE3	2.20	0.41
1:A:447:LEU:HD23	1:A:447:LEU:HA	1.95	0.41
1:A:274:LYS:HE3	1:A:274:LYS:HB2	1.41	0.41
1:C:129:LEU:HD22	1:C:296:LEU:HD23	2.02	0.41
1:A:144:LYS:HB2	1:A:144:LYS:HE2	1.92	0.41
1:A:129:LEU:HD23	1:A:299:VAL:HG21	2.03	0.41
1:D:222:ARG:NH2	8:D:2163:HOH:O	2.53	0.41
1:A:189:ARG:HA	1:A:212:PRO:HD2	2.02	0.41
1:B:174:HIS:HE1	8:B:2081:HOH:O	2.03	0.41
1:C:421:ASP:C	1:C:421:ASP:OD1	2.59	0.41
1:D:224[A]:ASN:ND2	1:D:252:ASN:OD1	2.54	0.41
1:B:482:GLU:HG3	1:B:484:MET:HE3	2.03	0.41
1:B:142:ASP:HA	1:B:143:PRO:HD3	1.94	0.41
1:D:302:LYS:H	1:D:318:ASN:HD21	1.69	0.41
1:C:485:GLU:HG3	1:C:486:LYS:HG2	2.03	0.41
3:B:1000:WPE:HAW1	3:B:1000:WPE:HAM2	1.67	0.40
1:A:331[B]:ARG:HB3	8:A:2264:HOH:O	2.21	0.40
1:D:400:MET:HG3	1:D:401:HIS:N	2.36	0.40
2:A:998:FAD:H1'1	2:A:998:FAD:H9	1.89	0.40
1:D:238:VAL:O	1:D:242:LEU:HG	2.21	0.40
1:A:48:LEU:HD11	1:A:114:PHE:HE2	1.86	0.40
1:D:228:ARG:HB3	1:D:228:ARG:HE	1.21	0.40
1:A:92:TRP:HB3	1:A:187:PRO:HD3	2.03	0.40
1:C:399:LEU:O	1:C:400:MET:C	2.60	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%)	477 (97%)	12 (2%)	1 (0%)	56 57
1	B	486/495 (98%)	469 (96%)	12 (2%)	5 (1%)	22 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	486/495 (98%)	458 (94%)	24 (5%)	4 (1%)	27	20
1	D	491/495 (99%)	473 (96%)	13 (3%)	5 (1%)	22	14
All	All	1953/1980 (99%)	1877 (96%)	61 (3%)	15 (1%)	30	20

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	132	LYS
1	A	352	ASN
1	C	28	GLY
1	B	306	LYS
1	B	354	PRO
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	396	PHE
1	D	480	LYS
1	B	45	TYR
1	C	55	VAL
1	C	298	ASN
1	D	55	VAL
1	B	55	VAL
1	B	349	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%)	385 (95%)	20 (5%)	35	31
1	B	400/407 (98%)	380 (95%)	20 (5%)	34	30
1	C	401/407 (98%)	379 (94%)	22 (6%)	30	26
1	D	404/407 (99%)	382 (95%)	22 (5%)	31	27
All	All	1610/1628 (99%)	1526 (95%)	84 (5%)	34	29

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	A	1	MET
1	A	57	CYS
1	A	60	LYS
1	A	99	LYS
1	A	228	ARG
1	A	238	VAL
1	A	251	THR
1	A	274	LYS
1	A	290	ARG
1	A	318	ASN
1	A	331[A]	ARG
1	A	331[B]	ARG
1	A	335	THR
1	A	353	LYS
1	A	387	GLU
1	A	400	MET
1	A	472	ARG
1	A	480	LYS
1	A	486	LYS
1	B	57	CYS
1	B	60	LYS
1	B	89	LYS
1	B	129	LEU
1	B	132	LYS
1	B	144	LYS
1	B	150	ARG
1	B	152	GLN
1	B	238	VAL
1	B	260	LEU
1	B	302	LYS
1	B	321	ASN
1	B	322	ILE
1	B	352	ASN
1	B	353	LYS
1	B	355	ARG
1	B	356	LYS
1	B	385	GLU
1	B	485	GLU
1	B	486	LYS
1	C	3	LYS
1	C	30	ARG
1	C	57	CYS

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Mol	Chain	Res	Type
1	C	60	LYS
1	C	99	LYS
1	C	129	LEU
1	C	132	LYS
1	C	150	ARG
1	C	152	GLN
1	C	154	ASP
1	C	224[A]	ASN
1	C	224[B]	ASN
1	C	248	GLU
1	C	260	LEU
1	C	262	THR
1	C	306	LYS
1	C	318	ASN
1	C	323	TYR
1	C	331	ARG
1	C	354	PRO
1	C	400	MET
1	C	446	ARG
1	D	57	CYS
1	D	60	LYS
1	D	89	LYS
1	D	94	LYS
1	D	99	LYS
1	D	129	LEU
1	D	131	SER
1	D	149	GLU
1	D	224[A]	ASN
1	D	224[B]	ASN
1	D	228	ARG
1	D	231	ASP
1	D	266	LYS
1	D	292	ASN
1	D	318	ASN
1	D	331[A]	ARG
1	D	331[B]	ARG
1	D	335	THR
1	D	472	ARG
1	D	480	LYS
1	D	482	GLU
1	D	485	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	318	ASN
1	B	72	HIS
1	B	107	ASN
1	B	174	HIS
1	B	224	ASN
1	B	310	GLN
1	B	352	ASN
1	B	359	HIS
1	C	72	HIS
1	C	107	ASN
1	C	310	GLN
1	C	318	ASN
1	C	359	HIS
1	D	68	GLN
1	D	72	HIS
1	D	107	ASN
1	D	152	GLN
1	D	252	ASN
1	D	254	ASN
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 32 ligands modelled in this entry, 22 are monoatomic - leaving 10 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	WPE	A	1000	-	31,31,31	2.06	9 (29%)	42,43,43	1.81	7 (16%)
6	MPD	A	1494	-	7,7,7	0.71	0	10,10,10	0.62	0
2	FAD	A	998	-	58,58,58	1.26	5 (8%)	85,89,89	2.09	17 (20%)
3	WPE	B	1000	-	31,31,31	1.97	6 (19%)	42,43,43	1.80	8 (19%)
2	FAD	B	998	-	58,58,58	1.34	8 (13%)	85,89,89	2.12	16 (18%)
3	WPE	C	1000	-	31,31,31	2.13	8 (25%)	42,43,43	1.79	10 (23%)
2	FAD	C	998	-	58,58,58	1.17	5 (8%)	85,89,89	2.05	16 (18%)
3	WPE	D	1000	-	31,31,31	2.03	8 (25%)	42,43,43	2.06	12 (28%)
7	MRD	D	1492	-	7,7,7	0.57	0	10,10,10	0.75	0
2	FAD	D	998	-	58,58,58	1.23	6 (10%)	85,89,89	2.22	17 (20%)

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	WPE	A	1000	-	-	1/12/30/30	0/2/4/4
6	MPD	A	1494	-	-	0/5/5/5	0/0/0/0
2	FAD	A	998	-	-	0/34/50/50	0/1/6/6
3	WPE	B	1000	-	-	0/12/30/30	0/2/4/4
2	FAD	B	998	-	-	0/34/50/50	0/1/6/6
3	WPE	C	1000	-	-	1/12/30/30	0/2/4/4
2	FAD	C	998	-	-	0/34/50/50	0/1/6/6
3	WPE	D	1000	-	-	0/12/30/30	0/2/4/4
7	MRD	D	1492	-	-	0/5/5/5	0/0/0/0
2	FAD	D	998	-	-	0/34/50/50	0/1/6/6

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1000	WPE	CAE-CAK	6.40	1.59	1.52
3	C	1000	WPE	CAV-NAU	6.36	1.40	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1000	WPE	CAV-NAU	6.35	1.40	1.29
2	A	998	FAD	C5X-N5	5.16	1.43	1.35
3	B	1000	WPE	CAE-CAK	5.05	1.58	1.52
3	D	1000	WPE	CAV-NAL	4.92	1.43	1.35
3	D	1000	WPE	CAJ-CAK	4.56	1.57	1.52
3	C	1000	WPE	CAV-NAL	4.48	1.42	1.35
3	D	1000	WPE	CAV-NAU	4.43	1.37	1.29
3	D	1000	WPE	CAE-CAK	4.24	1.57	1.52
3	A	1000	WPE	CAV-NAU	4.13	1.37	1.29
3	B	1000	WPE	CAV-NAL	3.95	1.41	1.35
2	B	998	FAD	C2B-C1B	-3.86	1.48	1.53
3	D	1000	WPE	CAW-CAV	3.71	1.55	1.49
2	C	998	FAD	C2A-N3A	3.66	1.39	1.32
3	C	1000	WPE	CAK-NAL	3.45	1.50	1.48
2	B	998	FAD	C6-C5X	-3.44	1.37	1.41
3	C	1000	WPE	CAJ-CAK	3.39	1.55	1.52
3	C	1000	WPE	CAW-CAV	3.39	1.55	1.49
2	B	998	FAD	C2A-N3A	3.36	1.38	1.32
2	A	998	FAD	C2A-N1A	3.35	1.40	1.33
2	D	998	FAD	C2A-N3A	3.18	1.38	1.32
3	A	1000	WPE	CAW-CAV	3.10	1.54	1.49
2	C	998	FAD	C2A-N1A	3.04	1.39	1.33
3	C	1000	WPE	CAM-NAL	3.02	1.51	1.46
2	D	998	FAD	C5X-N5	2.99	1.39	1.35
3	A	1000	WPE	CAM-NAL	2.94	1.51	1.46
2	D	998	FAD	C1'-N10	2.86	1.51	1.48
2	B	998	FAD	C2A-N1A	2.86	1.39	1.33
3	A	1000	WPE	CAY-CAP	2.85	1.56	1.50
3	A	1000	WPE	CAC-CAF	2.79	1.45	1.39
3	A	1000	WPE	CAA-CAD	2.78	1.45	1.39
3	D	1000	WPE	CAY-CAP	2.78	1.56	1.50
3	B	1000	WPE	CAW-CAV	2.70	1.54	1.49
2	B	998	FAD	C5X-N5	2.63	1.39	1.35
2	C	998	FAD	O4-C4	2.63	1.29	1.24
2	D	998	FAD	C5'-C4'	2.56	1.55	1.51
3	C	1000	WPE	CAY-CAP	2.43	1.55	1.50
2	A	998	FAD	C8A-N9A	2.33	1.40	1.36
2	A	998	FAD	C2A-N3A	2.32	1.36	1.32
2	C	998	FAD	C5X-N5	2.28	1.38	1.35
2	D	998	FAD	C2A-N1A	2.28	1.38	1.33
3	C	1000	WPE	CAI-CAH	2.27	1.42	1.38
3	A	1000	WPE	CAJ-CAK	-2.24	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	998	FAD	O4-C4	2.24	1.28	1.24
2	A	998	FAD	C4A-N9A	-2.17	1.34	1.37
2	B	998	FAD	C1'-N10	2.12	1.50	1.48
2	B	998	FAD	P-O3P	-2.11	1.56	1.59
2	B	998	FAD	C4X-C10	-2.10	1.37	1.40
2	C	998	FAD	C10-N1	2.08	1.39	1.35
3	B	1000	WPE	CAY-CAP	2.07	1.55	1.50
3	D	1000	WPE	CAI-CAH	2.06	1.41	1.38
3	B	1000	WPE	CAD-CAE	2.04	1.42	1.39
3	A	1000	WPE	CAC-CAB	2.03	1.43	1.37
3	D	1000	WPE	OAZ-CBB	2.00	1.39	1.35

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	998	FAD	N3A-C2A-N1A	-12.48	118.28	128.71
2	A	998	FAD	N3A-C2A-N1A	-11.64	118.98	128.71
2	B	998	FAD	N3A-C2A-N1A	-11.57	119.04	128.71
2	C	998	FAD	N3A-C2A-N1A	-10.22	120.17	128.71
2	D	998	FAD	C4X-N5-C5X	7.48	125.10	116.69
2	B	998	FAD	O4B-C1B-N9A	-6.53	102.36	108.44
3	D	1000	WPE	CBB-OAZ-CAY	-6.39	105.08	106.42
2	B	998	FAD	C1'-N10-C9A	6.22	124.92	118.87
2	C	998	FAD	C4X-N5-C5X	6.04	123.48	116.69
3	A	1000	WPE	CBB-OAZ-CAY	-5.77	105.21	106.42
3	B	1000	WPE	CBB-OAZ-CAY	-5.60	105.25	106.42
3	C	1000	WPE	CBB-OAZ-CAY	-5.49	105.27	106.42
2	A	998	FAD	O4B-C1B-N9A	-5.18	103.62	108.44
2	C	998	FAD	O4B-C1B-N9A	-5.11	103.69	108.44
2	D	998	FAD	C2-N1-C10	4.94	119.96	114.98
3	D	1000	WPE	CAS-CAT-CAJ	4.79	123.84	119.56
2	A	998	FAD	C2-N1-C10	4.79	119.81	114.98
2	D	998	FAD	C4X-C10-N1	-4.75	117.98	122.73
2	C	998	FAD	C2-N1-C10	4.69	119.70	114.98
2	A	998	FAD	C4X-N5-C5X	4.45	121.69	116.69
2	D	998	FAD	C10-C4X-N5	-4.41	115.10	120.45
3	C	1000	WPE	OAZ-CBB-CBA	-4.40	108.08	111.53
3	D	1000	WPE	CAW-CAV-NAL	4.21	122.89	117.85
3	B	1000	WPE	CAM-CAN-NAO	-4.15	103.81	111.59
3	C	1000	WPE	CAE-CAK-NAL	-4.14	105.25	111.54
2	C	998	FAD	N3A-C4A-N9A	4.07	132.78	125.43
2	A	998	FAD	C4X-C10-N1	-4.04	118.69	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	998	FAD	C2-N1-C10	3.90	118.90	114.98
3	B	1000	WPE	OAZ-CBB-CBA	-3.87	108.50	111.53
2	C	998	FAD	C4B-O4B-C1B	-3.81	105.61	109.75
3	A	1000	WPE	OAZ-CBB-CBA	-3.79	108.56	111.53
3	A	1000	WPE	CAE-CAK-NAL	-3.78	105.80	111.54
3	A	1000	WPE	CAH-CAI-CAJ	-3.77	115.85	120.08
3	A	1000	WPE	CAM-CAN-NAO	-3.56	104.91	111.59
2	D	998	FAD	N3A-C4A-N9A	3.54	131.83	125.43
2	B	998	FAD	N3A-C4A-N9A	3.53	131.81	125.43
2	D	998	FAD	C4-C4X-C10	3.42	122.47	116.95
3	D	1000	WPE	OAZ-CBB-CBA	-3.41	108.86	111.53
3	D	1000	WPE	CAT-NAU-CAV	3.41	122.68	118.38
2	A	998	FAD	C2A-N1A-C6A	3.38	124.87	118.77
2	D	998	FAD	O4B-C1B-N9A	-3.34	105.33	108.44
2	B	998	FAD	C4X-N5-C5X	3.23	120.32	116.69
3	B	1000	WPE	CAY-CAP-NAO	-3.22	111.69	116.18
3	B	1000	WPE	CAW-CAV-NAL	3.17	121.64	117.85
3	B	1000	WPE	CAE-CAK-NAL	-3.12	106.80	111.54
2	A	998	FAD	C4X-C10-N10	3.08	122.04	120.51
3	D	1000	WPE	CAE-CAK-NAL	-3.07	106.88	111.54
2	A	998	FAD	C1'-N10-C9A	3.06	121.84	118.87
2	C	998	FAD	C4-C4X-C10	3.03	121.84	116.95
3	A	1000	WPE	CAS-CAT-CAJ	3.01	122.25	119.56
2	A	998	FAD	C4-C4X-C10	2.97	121.75	116.95
2	A	998	FAD	N3A-C4A-N9A	2.97	130.79	125.43
2	D	998	FAD	C2A-N1A-C6A	2.96	124.12	118.77
3	C	1000	WPE	CAY-CAP-NAO	2.96	120.31	116.18
2	B	998	FAD	C4A-C5A-N7A	-2.93	107.02	109.52
3	C	1000	WPE	CAT-NAU-CAV	2.92	122.06	118.38
2	D	998	FAD	O2B-C2B-C1B	-2.90	102.46	111.23
2	B	998	FAD	C1'-N10-C10	-2.90	115.06	119.17
2	A	998	FAD	C2B-C1B-N9A	2.89	120.69	113.27
2	C	998	FAD	C4A-C5A-N7A	-2.87	107.06	109.52
3	D	1000	WPE	CAM-CAN-NAO	-2.86	106.22	111.59
2	C	998	FAD	C4X-C10-N1	-2.86	119.87	122.73
2	B	998	FAD	O4B-C1B-C2B	-2.81	102.46	106.77
2	B	998	FAD	C5X-C9A-N10	2.77	119.53	116.80
2	B	998	FAD	O2A-PA-O3P	2.74	118.13	105.14
2	C	998	FAD	N7A-C8A-N9A	-2.73	106.64	114.36
2	D	998	FAD	C4-N3-C2	-2.73	119.80	125.39
3	C	1000	WPE	CAE-CAK-CAJ	-2.72	107.73	112.54
2	A	998	FAD	C4-N3-C2	-2.70	119.85	125.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	998	FAD	C4A-C5A-N7A	-2.65	107.25	109.52
2	A	998	FAD	C9A-N10-C10	-2.65	119.17	121.77
3	D	1000	WPE	NAL-CAV-NAU	-2.64	119.96	123.33
2	A	998	FAD	O2'-C2'-C3'	2.62	115.57	109.05
2	A	998	FAD	C5X-C9A-N10	2.58	119.35	116.80
2	D	998	FAD	N7A-C8A-N9A	-2.56	107.10	114.36
2	C	998	FAD	C2'-C1'-N10	-2.56	109.05	112.45
2	C	998	FAD	C5A-C4A-N3A	-2.52	120.22	125.70
2	C	998	FAD	C8A-N7A-C5A	2.47	111.24	103.58
2	B	998	FAD	C3B-C2B-C1B	2.43	104.72	100.91
2	B	998	FAD	N7A-C8A-N9A	-2.43	107.48	114.36
3	D	1000	WPE	CAY-CAP-NAO	-2.42	112.81	116.18
2	A	998	FAD	O4B-C1B-C2B	-2.34	103.18	106.77
2	C	998	FAD	C5X-C9A-N10	2.33	119.10	116.80
3	C	1000	WPE	CAR-CAH-CAI	-2.27	118.39	121.54
2	B	998	FAD	C8A-N7A-C5A	2.23	110.48	103.58
2	D	998	FAD	C8A-N7A-C5A	2.22	110.45	103.58
3	C	1000	WPE	CAW-CAV-NAL	2.21	120.49	117.85
3	C	1000	WPE	CAJ-CAK-NAL	2.20	113.89	110.65
3	B	1000	WPE	NAL-CAV-NAU	-2.18	120.54	123.33
2	C	998	FAD	C2B-C1B-N9A	2.17	118.85	113.27
2	D	998	FAD	C5A-C4A-N3A	-2.15	121.02	125.70
2	D	998	FAD	C2A-N3A-C4A	2.14	120.11	114.01
2	D	998	FAD	C1B-N9A-C4A	-2.12	122.97	126.64
2	B	998	FAD	C2B-C1B-N9A	2.12	118.72	113.27
2	C	998	FAD	C9A-C5X-N5	-2.11	119.13	122.37
2	A	998	FAD	O2B-C2B-C1B	-2.10	104.88	111.23
3	D	1000	WPE	CAW-CAV-NAU	-2.09	117.15	119.68
3	D	1000	WPE	CAR-CAH-CAI	2.09	124.43	121.54
3	B	1000	WPE	CAE-CAK-CAJ	-2.09	108.85	112.54
3	D	1000	WPE	CAJ-CAT-NAU	-2.05	120.08	122.22
3	C	1000	WPE	CAI-CAH-CL	2.05	121.68	119.14
2	B	998	FAD	C2A-N3A-C4A	2.04	119.81	114.01
3	A	1000	WPE	CAW-CAV-NAL	2.03	120.28	117.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1000	WPE	CAX-CAY-CAP-NAO
3	A	1000	WPE	CAX-CAY-CAP-NAO

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	490/495 (98%)	-0.30	8 (1%) 68 72	12, 20, 36, 51	0
1	B	486/495 (98%)	0.07	23 (4%) 30 33	15, 27, 48, 60	0
1	C	484/495 (97%)	0.09	26 (5%) 25 27	14, 27, 56, 68	0
1	D	489/495 (98%)	-0.25	7 (1%) 72 76	14, 23, 36, 56	0
All	All	1949/1980 (98%)	-0.10	64 (3%) 45 49	12, 24, 49, 68	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	479	VAL	4.6
1	C	319	VAL	3.9
1	C	8	VAL	3.6
1	B	322	ILE	3.4
1	C	32	ALA	3.4
1	A	488	PRO	3.2
1	C	296	LEU	3.2
1	B	384	LYS	3.1
1	B	299	VAL	3.1
1	C	30	ARG	3.0
1	A	305	PRO	3.0
1	B	487	LEU	2.9
1	C	7	LEU	2.9
1	C	300	GLY	2.8
1	C	123	PHE	2.8
1	B	488	PRO	2.7
1	B	352	ASN	2.7
1	D	478	TYR	2.7
1	B	479	VAL	2.6
1	D	483	LYS	2.5
1	D	484	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	305	PRO	2.5
1	C	120	LEU	2.5
1	B	136	VAL	2.5
1	C	318	ASN	2.5
1	C	384	LYS	2.4
1	C	322	ILE	2.4
1	C	382	ALA	2.4
1	C	297	GLY	2.4
1	A	480	LYS	2.4
1	B	388	LYS	2.4
1	D	305	PRO	2.3
1	B	158	LEU	2.3
1	B	484	MET	2.3
1	C	481	GLY	2.3
1	C	130	GLU	2.3
1	A	306	LYS	2.3
1	B	480	LYS	2.3
1	D	480	LYS	2.3
1	A	387	GLU	2.3
1	D	387	GLU	2.3
1	A	437	ILE	2.3
1	B	486	LYS	2.2
1	B	129	LEU	2.2
1	C	131	SER	2.2
1	B	385	GLU	2.2
1	B	8	VAL	2.2
1	B	147	VAL	2.2
1	C	323	TYR	2.2
1	A	438	ILE	2.2
1	C	350	PHE	2.2
1	B	150	ARG	2.2
1	B	319	VAL	2.2
1	A	352	ASN	2.1
1	C	136	VAL	2.1
1	C	301	VAL	2.1
1	C	381	VAL	2.1
1	B	296	LEU	2.1
1	C	129	LEU	2.1
1	C	305	PRO	2.1
1	C	352	ASN	2.1
1	B	23	ALA	2.0
1	B	323	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	20	GLY	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	MPD	A	1494	8/8	0.22	18.46	34,39,41,43	0
7	MRD	D	1492	8/8	0.18	6.89	39,42,44,44	0
3	WPE	D	1000	28/28	0.13	2.14	17,25,60,61	0
5	CL	A	1492	1/1	0.11	1.23	26,26,26,26	0
3	WPE	C	1000	28/28	0.17	0.97	40,49,82,83	0
4	NA	A	1489	1/1	0.15	0.67	26,26,26,26	0
5	CL	A	1493	1/1	0.11	0.67	35,35,35,35	0
2	FAD	D	998	53/53	0.10	0.57	11,16,19,20	0
5	CL	B	1494	1/1	0.12	0.44	33,33,33,33	0
3	WPE	B	1000	28/28	0.13	0.33	29,33,62,63	0
5	CL	B	1491	1/1	0.10	0.26	24,24,24,24	0
5	CL	D	1489	1/1	0.11	0.25	21,21,21,21	0
2	FAD	A	998	53/53	0.10	0.22	8,15,18,20	0
3	WPE	A	1000	28/28	0.11	0.15	15,24,53,54	0
2	FAD	B	998	53/53	0.13	0.07	15,24,37,39	0
4	NA	B	1489	1/1	0.11	-0.47	37,37,37,37	0
2	FAD	C	998	53/53	0.10	-0.49	16,26,36,38	0
5	CL	D	1488	1/1	0.09	-0.73	32,32,32,32	0
5	CL	A	1490	1/1	0.07	-0.74	24,24,24,24	0
5	CL	C	1489	1/1	0.16	-0.77	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CL	A	1491	1/1	0.07	-0.84	22,22,22,22	0
5	CL	C	1492	1/1	0.06	-0.89	34,34,34,34	0
5	CL	D	1490	1/1	0.09	-0.94	39,39,39,39	0
5	CL	C	1488	1/1	0.06	-0.94	39,39,39,39	0
5	CL	C	1490	1/1	0.06	-1.05	24,24,24,24	0
5	CL	C	1491	1/1	0.08	-1.22	42,42,42,42	0
5	CL	B	1492	1/1	0.06	-1.37	40,40,40,40	0
4	NA	D	1487	1/1	0.08	-1.48	33,33,33,33	0
5	CL	D	1491	1/1	0.07	-1.67	36,36,36,36	0
5	CL	B	1490	1/1	0.04	-1.78	27,27,27,27	0
4	NA	C	1487	1/1	0.06	-2.83	26,26,26,26	0
5	CL	B	1493	1/1	0.10	-5.26	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.