W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:21 AM GMT

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PDB ID	:	2WPF
Title	:	TRYPANOSOMA BRUCEI TRYPANOTHIONE REDUCTASE IN COMPLEX WITH 3,4-DIHYDROQUINAZOLINE INHIBITOR (DDD00085762)
Authors	:	Alphey, M.S.; Patterson, S.; Fairlamb, A.H.
Deposited on	:	2009-08-06
Resolution	:	1.90 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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.
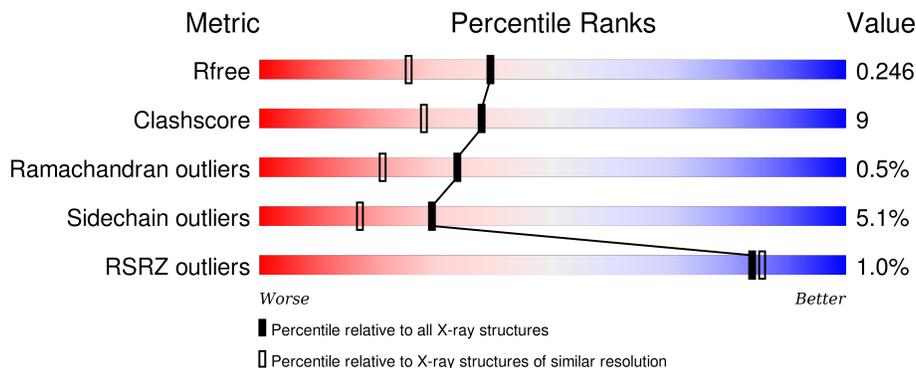
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	495	77% ... 19% ··
1	B	495	76% ... 20% ··
1	C	495	76% ... 21% ··
1	D	495	80% ... 17% ··

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	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 (i)

There are 6 unique types of molecules in this entry. The entry contains 16503 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called TRYPANOTHIONE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total 3733	C 2374	N 636	O 702	S 21	0	2	0
1	B	487	Total 3702	C 2353	N 631	O 699	S 19	0	2	0
1	C	487	Total 3716	C 2364	N 630	O 703	S 19	0	3	0
1	D	491	Total 3737	C 2376	N 635	O 706	S 20	0	2	0

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: $C_{27}H_{33}N_9O_{15}P_2$).
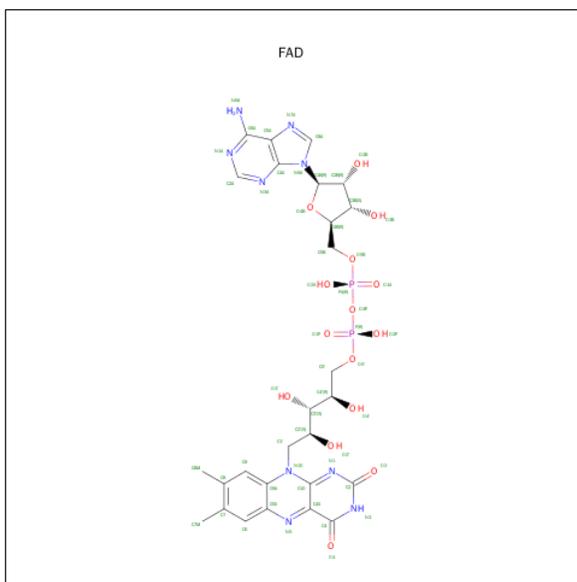
FAD

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)QUINAZOLIN-3(4H)-YL]-N,N-DIMETHYLPROPAN-1-AMINE (three-letter code: WPF) (formula: $C_{21}H_{26}ClN_3$).

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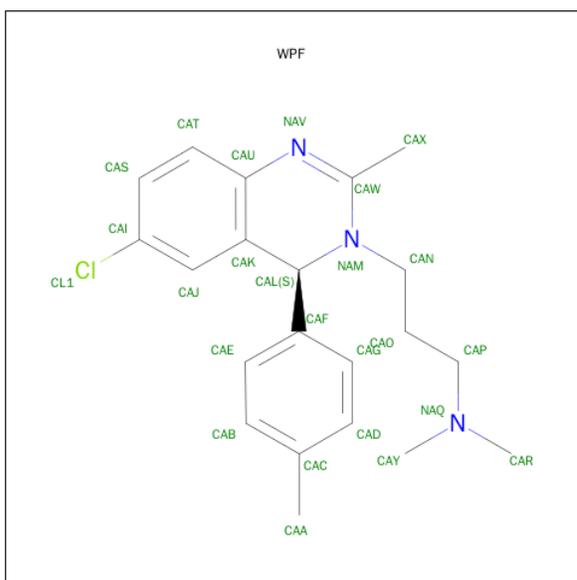
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 25	C 21	Cl 1	N 3		0	0
3	B	1	Total 25	C 21	Cl 1	N 3		0	0
3	C	1	Total 25	C 21	Cl 1	N 3		0	0
3	D	1	Total 25	C 21	Cl 1	N 3		0	0

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

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

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

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

- Molecule 6 is water.

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

3 Residue-property plots (i)

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

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M113 F114 G119 L120 D121 F122 F123 L124 S128 I129 E130 S131 K132 N133 V134 V135 V136 E139 D142 P143 K144 S145 Q152 A153 I156 L157 T160 G171 I176 E180 Y183 L184 P185 E186 R189 Y210 R228 D231 I234 R235 K240 Q241

V258 S259 L260 N261 T262 D263 H267 V268 T275 V299 G300 V301 K302 P305 K306 V311 S315 N318 V319 P320 N321 I322 I325 I328 T329 D330 T335 P336 G342 L345 N352 K353 P354 H359 P370 Y392 T397 N402 I403 S404 K410

L430 I438 V441 G442 V443 R446 L447 D453 F454 Y455 A465 E466 E467 L468 R472 K486 L487 P488 D489 SER ASN LEU

● Molecule 1: TRYPANOTHIONE REDUCTASE

Chain D:

%
80%   17%

G-2 V8 S14 E18 A19 G20 W21 K29 R30 V31 A32 V33 H40 G41 C52 V55 G56 C57 K60 H72 E75 W81 K89 K94 L95 K99 A102 V103 L104 N107 K108 V136 V147 E149 A153 D154 T160 Y183

E186 R189 R190 V191 Y210 K211 P212 K216 V217 Y221 R222 N223 N224 D231 E237 V238 E248 N254 L260 N261 K266 E271 D277 V278 D279 R290 T291 N292 G300 V301 K302 I303 T304 P305 K306 N318 N321 I328 R331 E341

F350 K353 H359 T360 R361 P370 P371 I372 S395 F396 M400 S404 F411 L429 L430 G431 Q439 R446 Y455 H461 L468 R472 T473 P474 Y477 K480 G481 E482 E485 K486 L487 P488 ASP SER ASN LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$<I/\sigma(I)>$ [1]	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^2)	19.0	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 50.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.43$, $<L^2> = 0.26$	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^2)	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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%)

The worst 5 of 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

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 278 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	490/495 (99%)	472 (96%)	16 (3%)	2 (0%)	39	27
1	B	487/495 (98%)	468 (96%)	16 (3%)	3 (1%)	30	17
1	C	488/495 (99%)	471 (96%)	15 (3%)	2 (0%)	39	27
1	D	491/495 (99%)	475 (97%)	13 (3%)	3 (1%)	30	17
All	All	1956/1980 (99%)	1886 (96%)	60 (3%)	10 (0%)	34	21

5 of 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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	405/407 (100%)	381 (94%)	24 (6%)	24	12
1	B	399/407 (98%)	382 (96%)	17 (4%)	35	23
1	C	403/407 (99%)	382 (95%)	21 (5%)	29	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	405/407 (100%)	382 (94%)	23 (6%)	25	13
All	All	1612/1628 (99%)	1527 (95%)	85 (5%)	29	16

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	407	LYS
1	C	99	LYS
1	D	331	ARG
1	B	480	LYS
1	C	57	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	107	ASN
1	C	318	ASN
1	D	321	ASN
1	C	152	GLN
1	C	310	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

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	-	25,27,27	2.00	6 (24%)	31,38,38	1.36	7 (22%)
2	FAD	A	998	-	48,58,58	1.24	5 (10%)	54,89,89	2.18	10 (18%)
3	WPF	B	1000	-	25,27,27	1.95	4 (16%)	31,38,38	1.52	5 (16%)
2	FAD	B	998	-	48,58,58	1.26	4 (8%)	54,89,89	2.60	11 (20%)
3	WPF	C	1000	-	25,27,27	2.31	6 (24%)	31,38,38	1.73	6 (19%)
2	FAD	C	998	-	48,58,58	1.14	3 (6%)	54,89,89	2.71	15 (27%)
3	WPF	D	1000	-	25,27,27	2.05	6 (24%)	31,38,38	1.42	3 (9%)
2	FAD	D	998	-	48,58,58	1.08	4 (8%)	54,89,89	2.18	10 (18%)

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	0/3/3/3
2	FAD	A	998	-	-	0/30/50/50	0/6/6/6
3	WPF	B	1000	-	-	0/10/26/26	0/3/3/3
2	FAD	B	998	-	-	0/30/50/50	0/6/6/6
3	WPF	C	1000	-	-	0/10/26/26	0/3/3/3
2	FAD	C	998	-	-	0/30/50/50	0/6/6/6
3	WPF	D	1000	-	-	0/10/26/26	0/3/3/3
2	FAD	D	998	-	-	0/30/50/50	0/6/6/6

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	998	FAD	C9A-C5X	-2.41	1.37	1.42
2	D	998	FAD	C5X-N5	2.00	1.38	1.35
3	A	1000	WPF	CAD-CAG	2.05	1.42	1.38
2	A	998	FAD	C2A-N3A	2.07	1.35	1.32
2	A	998	FAD	C4A-N3A	2.13	1.38	1.35

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	998	FAD	N3A-C2A-N1A	-13.09	118.87	128.89
2	B	998	FAD	N3A-C2A-N1A	-10.88	120.56	128.89
2	A	998	FAD	N3A-C2A-N1A	-10.17	121.11	128.89
2	D	998	FAD	N3A-C2A-N1A	-8.58	122.32	128.89
2	B	998	FAD	C4X-C4-N3	-5.97	115.43	123.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	WPF	4	0
3	B	1000	WPF	3	0
2	B	998	FAD	1	0
3	C	1000	WPF	8	0
3	D	1000	WPF	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	490/495 (98%)	-0.40	3 (0%)	90	91	9, 19, 33, 46	0
1	B	487/495 (98%)	-0.24	5 (1%)	84	86	13, 24, 41, 53	0
1	C	487/495 (98%)	-0.14	9 (1%)	71	74	12, 24, 45, 57	0
1	D	491/495 (99%)	-0.38	3 (0%)	90	91	10, 20, 33, 47	0
All	All	1955/1980 (98%)	-0.29	20 (1%)	84	86	9, 21, 41, 57	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	352	ASN	4.3
1	B	352	ASN	4.1
1	C	306	LYS	3.6
1	C	305	PRO	3.5
1	D	305	PRO	3.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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

wwPDB X-ray Structure Validation Summary Report

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
3	WPF	C	1000	25/25	0.81	0.27	5.68	48,62,66,67	0
3	WPF	D	1000	25/25	0.92	0.15	4.85	25,32,43,46	0
3	WPF	B	1000	25/25	0.90	0.18	3.18	36,41,54,55	0
3	WPF	A	1000	25/25	0.91	0.16	3.00	22,30,47,48	0
5	BR	B	1491	1/1	0.95	0.15	0.79	69,69,69,69	0
4	CL	B	1489	1/1	0.99	0.10	0.46	17,17,17,17	0
4	CL	A	1489	1/1	0.99	0.10	0.43	17,17,17,17	0
2	FAD	D	998	53/53	0.98	0.07	-0.17	11,14,18,19	0
2	FAD	B	998	53/53	0.97	0.08	-0.40	15,21,27,28	0
4	CL	A	1490	1/1	0.99	0.09	-0.42	19,19,19,19	0
4	CL	B	1490	1/1	1.00	0.07	-0.60	18,18,18,18	0
2	FAD	C	998	53/53	0.98	0.07	-0.77	13,21,27,28	0
4	CL	C	1490	1/1	0.99	0.08	-0.78	15,15,15,15	0
2	FAD	A	998	53/53	0.98	0.07	-0.83	2,12,16,17	0
5	BR	D	1489	1/1	0.94	0.09	-1.01	66,66,66,66	0
4	CL	C	1491	1/1	0.98	0.04	-1.32	22,22,22,22	0
5	BR	D	1490	1/1	1.00	0.02	-2.36	36,36,36,36	0
4	CL	A	1491	1/1	0.98	0.04	-	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.