



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2019 – 11:17 PM EDT

PDB ID : 6GCP
Title : Trypanosoma brucei PTR1 in complex with inhibitor 2d (F186)
Authors : Pozzi, C.; Landi, G.; Mangani, S.
Deposited on : 2018-04-18
Resolution : 1.52 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

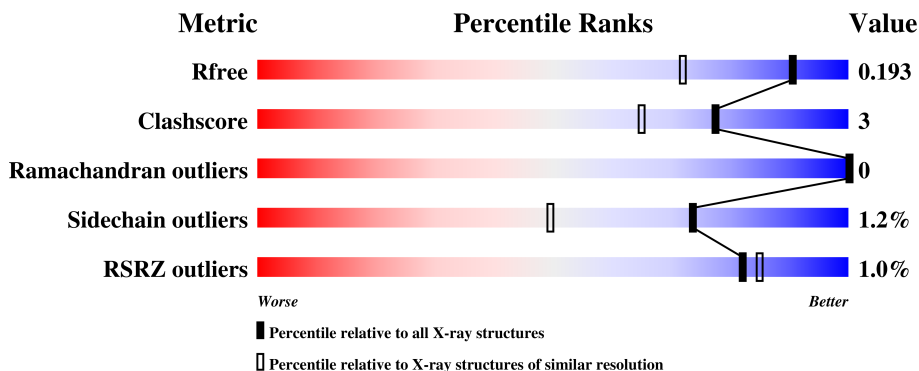
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.52 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}	111664	3365 (1.54-1.50)
Clashscore	122126	3586 (1.54-1.50)
Ramachandran outliers	120053	3504 (1.54-1.50)
Sidechain outliers	120020	3502 (1.54-1.50)
RSRZ outliers	108989	3301 (1.54-1.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div style="width: 81%;"></div> <div style="width: 6%;"></div> <div style="width: 13%;"></div> </div> <div>81% 6% 13%</div>
1	B	288	<div> <div style="width: 80%;"></div> <div style="width: 7%;"></div> <div style="width: 13%;"></div> </div> <div>80% 7% 13%</div>
1	C	288	<div> <div style="width: 80%;"></div> <div style="width: 7%;"></div> <div style="width: 13%;"></div> </div> <div>80% 7% 13%</div>
1	D	288	<div> <div style="width: 79%;"></div> <div style="width: 8%;"></div> <div style="width: 13%;"></div> </div> <div>79% 8% 13%</div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8831 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 Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	7	0
			1892	1192	333	356	11			
1	B	252	Total	C	N	O	S	0	8	0
			1893	1198	327	356	12			
1	C	251	Total	C	N	O	S	0	10	0
			1885	1191	327	355	12			
1	D	250	Total	C	N	O	S	0	14	0
			1921	1217	330	362	12			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP O76290
A	-18	GLY	-	expression tag	UNP O76290
A	-17	SER	-	expression tag	UNP O76290
A	-16	SER	-	expression tag	UNP O76290
A	-15	HIS	-	expression tag	UNP O76290
A	-14	HIS	-	expression tag	UNP O76290
A	-13	HIS	-	expression tag	UNP O76290
A	-12	HIS	-	expression tag	UNP O76290
A	-11	HIS	-	expression tag	UNP O76290
A	-10	HIS	-	expression tag	UNP O76290
A	-9	SER	-	expression tag	UNP O76290
A	-8	SER	-	expression tag	UNP O76290
A	-7	GLY	-	expression tag	UNP O76290
A	-6	LEU	-	expression tag	UNP O76290
A	-5	VAL	-	expression tag	UNP O76290
A	-4	PRO	-	expression tag	UNP O76290
A	-3	ARG	-	expression tag	UNP O76290
A	-2	GLY	-	expression tag	UNP O76290
A	-1	SER	-	expression tag	UNP O76290
A	0	HIS	-	expression tag	UNP O76290
B	-19	MET	-	initiating methionine	UNP O76290

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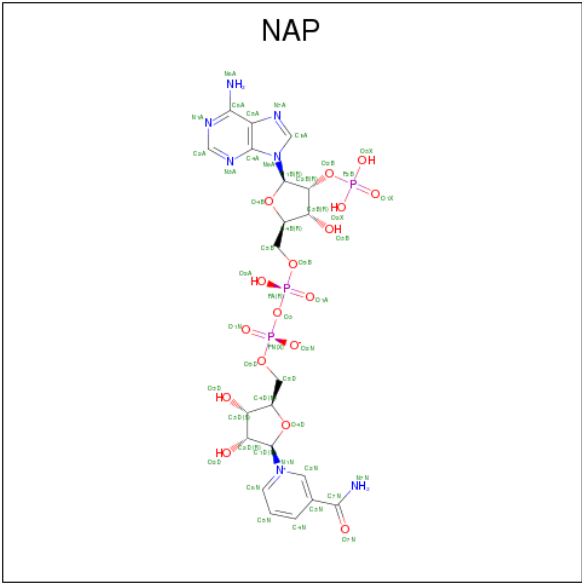
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	UNP O76290
B	-12	HIS	-	expression tag	UNP O76290
B	-11	HIS	-	expression tag	UNP O76290
B	-10	HIS	-	expression tag	UNP O76290
B	-9	SER	-	expression tag	UNP O76290
B	-8	SER	-	expression tag	UNP O76290
B	-7	GLY	-	expression tag	UNP O76290
B	-6	LEU	-	expression tag	UNP O76290
B	-5	VAL	-	expression tag	UNP O76290
B	-4	PRO	-	expression tag	UNP O76290
B	-3	ARG	-	expression tag	UNP O76290
B	-2	GLY	-	expression tag	UNP O76290
B	-1	SER	-	expression tag	UNP O76290
B	0	HIS	-	expression tag	UNP O76290
C	-19	MET	-	initiating methionine	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290
C	-16	SER	-	expression tag	UNP O76290
C	-15	HIS	-	expression tag	UNP O76290
C	-14	HIS	-	expression tag	UNP O76290
C	-13	HIS	-	expression tag	UNP O76290
C	-12	HIS	-	expression tag	UNP O76290
C	-11	HIS	-	expression tag	UNP O76290
C	-10	HIS	-	expression tag	UNP O76290
C	-9	SER	-	expression tag	UNP O76290
C	-8	SER	-	expression tag	UNP O76290
C	-7	GLY	-	expression tag	UNP O76290
C	-6	LEU	-	expression tag	UNP O76290
C	-5	VAL	-	expression tag	UNP O76290
C	-4	PRO	-	expression tag	UNP O76290
C	-3	ARG	-	expression tag	UNP O76290
C	-2	GLY	-	expression tag	UNP O76290
C	-1	SER	-	expression tag	UNP O76290
C	0	HIS	-	expression tag	UNP O76290
D	-19	MET	-	initiating methionine	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP O76290
D	-15	HIS	-	expression tag	UNP O76290
D	-14	HIS	-	expression tag	UNP O76290
D	-13	HIS	-	expression tag	UNP O76290
D	-12	HIS	-	expression tag	UNP O76290
D	-11	HIS	-	expression tag	UNP O76290
D	-10	HIS	-	expression tag	UNP O76290
D	-9	SER	-	expression tag	UNP O76290
D	-8	SER	-	expression tag	UNP O76290
D	-7	GLY	-	expression tag	UNP O76290
D	-6	LEU	-	expression tag	UNP O76290
D	-5	VAL	-	expression tag	UNP O76290
D	-4	PRO	-	expression tag	UNP O76290
D	-3	ARG	-	expression tag	UNP O76290
D	-2	GLY	-	expression tag	UNP O76290
D	-1	SER	-	expression tag	UNP O76290
D	0	HIS	-	expression tag	UNP O76290

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



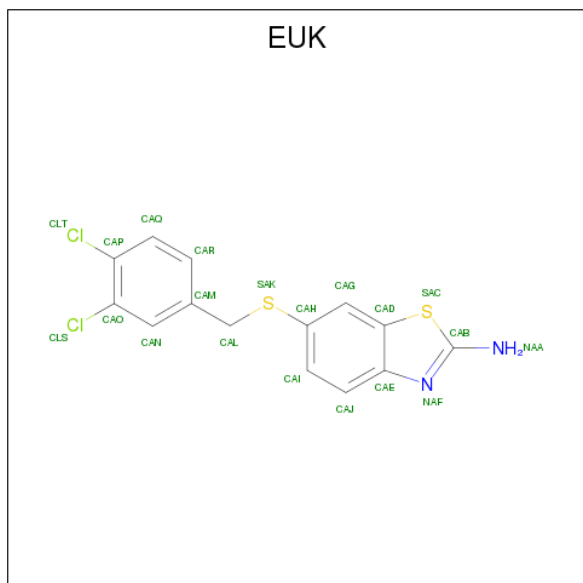
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
2	B	1	Total 48	C 21	N 7	O 17	P 3	0	0

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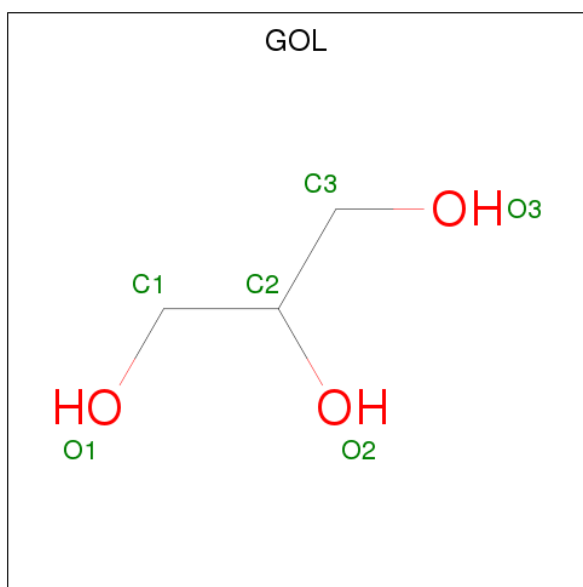
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 6-[(3,4-dichlorophenyl)methylsulfanyl]-1,3-benzothiazol-2-amine (three-letter code: EUK) (formula: $C_{14}H_{10}Cl_2N_2S_2$).



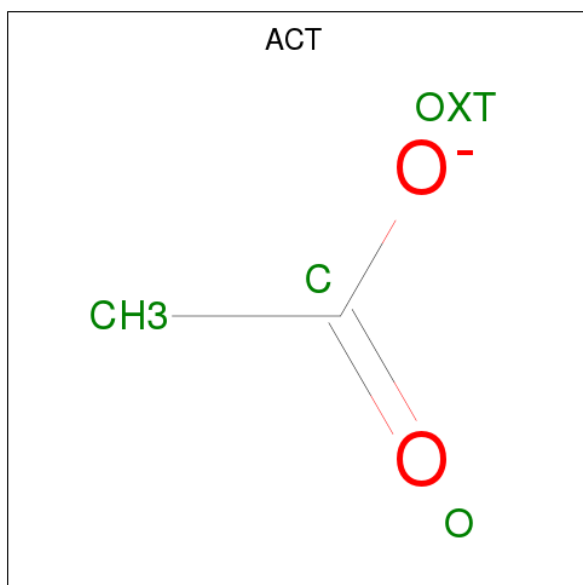
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	1
			40	28	4	4	4		
3	B	1	Total	C	Cl	N	S	0	0
			20	14	2	2	2		
3	C	1	Total	C	Cl	N	S	0	1
			40	28	4	4	4		
3	D	1	Total	C	Cl	N	S	0	1
			40	28	4	4	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	209	Total	O	0	4
			213	213		
6	B	238	Total	O	0	8
			246	246		
6	C	201	Total	O	0	4
			204	204		
6	D	208	Total	O	0	7
			213	213		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.87Å 90.37Å 82.93Å 90.00° 115.68° 90.00°	Depositor
Resolution (Å)	67.48 – 1.52 67.47 – 1.52	Depositor EDS
% Data completeness (in resolution range)	97.7 (67.48-1.52) 97.7 (67.47-1.52)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 1.52Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.166 , 0.193 0.167 , 0.193	Depositor DCC
R_{free} test set	7581 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8831	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.7829e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAP, EUK, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.75	0/1934	0.84	0/2626
1	B	0.77	0/1941	0.87	0/2636
1	C	0.74	0/1936	0.81	0/2631
1	D	0.77	0/1984	0.81	0/2692
All	All	0.76	0/7795	0.83	0/10585

There are no bond length outliers.

There are no bond angle outliers.

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	1892	0	1912	14	0
1	B	1893	0	1917	17	0
1	C	1885	0	1900	16	0
1	D	1921	0	1961	18	0
2	A	48	0	25	0	0
2	B	48	0	25	2	0
2	C	48	0	25	0	0
2	D	48	0	25	1	0
3	A	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	1	0
3	C	40	0	0	1	0
3	D	40	0	0	2	0
4	A	6	0	8	0	0
4	B	12	0	16	1	0
4	C	6	0	8	0	0
5	B	8	0	6	1	0
6	A	213	0	0	0	0
6	B	246	0	0	0	0
6	C	204	0	0	0	0
6	D	213	0	0	1	0
All	All	8831	0	7828	50	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 3.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140[B]:GLN:NE2	1:C:104:GLN:H	1.82	0.77
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.19	0.76
1:C:210:PRO:HG2	3:C:302[A]:EUK:CLS	2.30	0.68
1:D:210:PRO:HG2	3:D:302[A]:EUK:CLS	2.32	0.67
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.31	0.66
1:C:236:GLN:HE21	1:D:250[B]:GLN:CG	2.09	0.65
1:A:210:PRO:HG2	3:A:302[A]:EUK:CLS	2.37	0.61
1:A:265:LEU:HB2	1:B:190[B]:LEU:HD21	1.84	0.60
1:C:236:GLN:HE21	1:D:250[B]:GLN:CD	2.05	0.60
1:D:213:MET:HE3	3:D:302[B]:EUK:CAQ	2.33	0.58
1:A:206[B]:VAL:HG23	1:A:263:LEU:HD22	1.85	0.57
1:B:210:PRO:HG2	3:B:302:EUK:CLS	2.42	0.56
1:A:140[B]:GLN:HE22	1:C:104:GLN:H	1.53	0.56
1:A:250:GLN:CD	1:B:236:GLN:HE21	2.10	0.55
1:A:2:GLU:HG2	1:A:86:ARG:HH11	1.73	0.53
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.90	0.52
1:D:206[A]:VAL:HG23	1:D:263:LEU:HD22	1.91	0.52
1:B:103:VAL:HG22	6:D:405:HOH:O	2.10	0.51
1:D:22[B]:LYS:HG2	1:D:242:ILE:HG13	1.92	0.51
1:C:228:GLY:HA3	1:C:230:ARG:NH1	2.25	0.51
1:D:219:ASP:HB3	1:D:223:ARG:NH1	2.26	0.50
1:C:9:THR:HA	1:C:33:HIS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136[B]:MET:HE1	1:D:116:VAL:HG21	1.94	0.50
1:C:247:GLY:HA2	1:C:250:GLN:HG3	1.93	0.49
1:A:9:THR:HA	1:A:33:HIS:HB3	1.94	0.49
1:B:15:ILE:HB	2:B:301:NAP:H51N	1.96	0.48
1:C:236:GLN:NE2	1:D:250[B]:GLN:CG	2.77	0.48
1:A:250:GLN:CG	1:B:236:GLN:HE21	2.28	0.46
1:B:102:LEU:O	1:D:136[B]:MET:HG3	2.16	0.46
1:B:138:PHE:O	1:B:142:GLN:HG2	2.16	0.46
1:C:206[A]:VAL:HG23	1:C:209:LEU:CD1	2.45	0.46
1:A:22:LYS:HG2	1:A:242:ILE:HG13	1.98	0.46
1:B:25:GLN:HG3	4:B:305:GOL:H32	1.98	0.45
1:C:265:LEU:HD11	1:D:254:GLY:HA3	1.98	0.45
1:B:116:VAL:HG21	1:D:136[B]:MET:HE1	1.98	0.45
1:D:35:HIS:HB2	2:D:301:NAP:C2A	2.47	0.44
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.98	0.44
1:A:2:GLU:HG2	1:A:86:ARG:NH1	2.33	0.44
1:B:9:THR:HA	1:B:33:HIS:HB3	2.00	0.43
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.99	0.43
1:B:104:GLN:H	1:D:140:GLN:HE22	1.66	0.42
1:B:65:ASN:HA	1:B:69:LEU:HD22	2.01	0.42
1:C:206[A]:VAL:HG23	1:C:209:LEU:HD11	2.02	0.42
1:A:116:VAL:HG21	1:C:136[B]:MET:HE1	2.02	0.42
1:B:206[A]:VAL:CG2	1:B:209:LEU:HD21	2.50	0.42
1:B:35:HIS:HB2	2:B:301:NAP:C2A	2.49	0.42
1:A:120:VAL:HG11	1:C:129[B]:ILE:HD13	2.02	0.41
1:D:247:GLY:HA2	1:D:250[A]:GLN:HG3	2.01	0.41
1:D:115:THR:OG1	1:D:117[B]:GLU:HG2	2.21	0.41
1:B:214:GLY:HA2	5:B:304:ACT:H1	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/288 (88%)	243 (96%)	9 (4%)	0	100	100
1	B	254/288 (88%)	246 (97%)	8 (3%)	0	100	100
1	C	255/288 (88%)	245 (96%)	10 (4%)	0	100	100
1	D	258/288 (90%)	249 (96%)	9 (4%)	0	100	100
All	All	1019/1152 (88%)	983 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	200/231 (87%)	196 (98%)	4 (2%)	58	26
1	B	200/231 (87%)	198 (99%)	2 (1%)	78	58
1	C	199/231 (86%)	197 (99%)	2 (1%)	78	58
1	D	206/231 (89%)	205 (100%)	1 (0%)	90	79
All	All	805/924 (87%)	796 (99%)	9 (1%)	74	54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	53	SER
1	A	141	ARG
1	A	164	VAL
1	B	164	VAL
1	B	210	PRO
1	C	131	PRO
1	C	141	ARG
1	D	2	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	B	65	ASN
1	B	236	GLN
1	C	236	GLN
1	D	179	HIS

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](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	NAP	A	301	-	43,52,52	1.35	4 (9%)	53,80,80	1.51	7 (13%)
3	EUK	A	302[A]	-	19,22,22	1.96	4 (21%)	25,31,31	1.70	7 (28%)
3	EUK	A	302[B]	-	19,22,22	2.05	5 (26%)	25,31,31	1.34	6 (24%)
4	GOL	A	303	-	5,5,5	0.50	0	5,5,5	0.33	0
2	NAP	B	301	-	43,52,52	1.29	5 (11%)	53,80,80	1.75	9 (16%)
3	EUK	B	302	-	19,22,22	2.33	7 (36%)	25,31,31	1.63	6 (24%)
5	ACT	B	303	-	1,3,3	1.05	0	0,3,3	0.00	-
5	ACT	B	304	-	1,3,3	2.33	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	B	305	-	5,5,5	0.45	0	5,5,5	0.81	0
4	GOL	B	306	-	5,5,5	0.42	0	5,5,5	0.45	0
2	NAP	C	301	-	43,52,52	1.37	5 (11%)	53,80,80	1.68	10 (18%)
3	EUK	C	302[A]	-	19,22,22	2.24	5 (26%)	25,31,31	1.33	6 (24%)
3	EUK	C	302[B]	-	19,22,22	1.97	3 (15%)	25,31,31	1.23	3 (12%)
4	GOL	C	303	-	5,5,5	1.48	1 (20%)	5,5,5	1.73	2 (40%)
2	NAP	D	301	-	43,52,52	1.47	5 (11%)	53,80,80	1.61	8 (15%)
3	EUK	D	302[A]	-	19,22,22	1.87	4 (21%)	25,31,31	1.54	7 (28%)
3	EUK	D	302[B]	-	19,22,22	1.81	3 (15%)	25,31,31	1.45	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	A	301	-	-	0/27/67/67	0/5/5/5
3	EUK	A	302[A]	-	-	0/5/5/5	0/3/3/3
3	EUK	A	302[B]	-	-	0/5/5/5	0/3/3/3
4	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
3	EUK	B	302	-	-	0/5/5/5	0/3/3/3
5	ACT	B	303	-	-	0/0/0/0	0/0/0/0
5	ACT	B	304	-	-	0/0/0/0	0/0/0/0
4	GOL	B	305	-	-	0/4/4/4	0/0/0/0
4	GOL	B	306	-	-	0/4/4/4	0/0/0/0
2	NAP	C	301	-	-	0/27/67/67	0/5/5/5
3	EUK	C	302[A]	-	-	0/5/5/5	0/3/3/3
3	EUK	C	302[B]	-	-	0/5/5/5	0/3/3/3
4	GOL	C	303	-	-	0/4/4/4	0/0/0/0
2	NAP	D	301	-	-	0/27/67/67	0/5/5/5
3	EUK	D	302[A]	-	-	0/5/5/5	0/3/3/3
3	EUK	D	302[B]	-	-	0/5/5/5	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302[B]	EUK	CAL-CAM	-5.11	1.39	1.51
3	D	302[B]	EUK	CAL-CAM	-5.04	1.39	1.51
3	C	302[B]	EUK	CAL-CAM	-4.91	1.40	1.51
3	B	302	EUK	CAL-CAM	-4.89	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	302[A]	EUK	CAL-CAM	-4.85	1.40	1.51
3	A	302[A]	EUK	CAL-CAM	-4.79	1.40	1.51
3	D	302[A]	EUK	CAL-CAM	-4.47	1.41	1.51
3	D	302[B]	EUK	CAJ-CAE	-3.92	1.35	1.41
3	C	302[B]	EUK	CAJ-CAE	-3.53	1.35	1.41
3	D	302[A]	EUK	CAJ-CAE	-3.45	1.35	1.41
3	A	302[A]	EUK	CAJ-CAE	-3.40	1.35	1.41
3	A	302[B]	EUK	CAJ-CAE	-3.19	1.36	1.41
3	C	302[A]	EUK	CAJ-CAE	-3.16	1.36	1.41
3	B	302	EUK	CAJ-CAE	-2.82	1.36	1.41
3	B	302	EUK	CAG-CAD	-2.18	1.33	1.38
3	D	302[A]	EUK	CAN-CAO	2.01	1.41	1.38
2	C	301	NAP	O4D-C1D	2.03	1.44	1.41
3	A	302[A]	EUK	CAJ-CAI	2.08	1.40	1.36
2	A	301	NAP	C2A-N1A	2.12	1.37	1.33
2	B	301	NAP	C4A-N3A	2.16	1.38	1.35
2	C	301	NAP	P2B-O2B	2.16	1.63	1.59
2	B	301	NAP	C6A-C5A	2.21	1.51	1.43
3	D	302[B]	EUK	CAH-SAK	2.22	1.81	1.76
2	C	301	NAP	C8A-N7A	2.30	1.38	1.34
2	D	301	NAP	O4D-C1D	2.31	1.44	1.41
5	B	304	ACT	CH3-C	2.33	1.51	1.48
3	B	302	EUK	CAJ-CAI	2.34	1.41	1.36
3	B	302	EUK	CAN-CAO	2.35	1.42	1.38
3	A	302[B]	EUK	CAH-SAK	2.39	1.81	1.76
4	C	303	GOL	O3-C3	2.41	1.52	1.42
2	B	301	NAP	O4D-C1D	2.76	1.45	1.41
2	D	301	NAP	C7N-N7N	2.87	1.38	1.33
2	A	301	NAP	P2B-O2B	2.89	1.64	1.59
3	C	302[A]	EUK	CAO-CLS	2.92	1.80	1.73
3	A	302[B]	EUK	CAO-CLS	2.99	1.80	1.73
3	B	302	EUK	CAO-CLS	3.12	1.81	1.73
2	B	301	NAP	C5A-C4A	3.16	1.47	1.40
2	D	301	NAP	C5A-C4A	3.17	1.47	1.40
2	B	301	NAP	C2A-N3A	3.20	1.37	1.32
2	A	301	NAP	C5A-C4A	3.32	1.48	1.40
3	C	302[A]	EUK	CAP-CLT	3.45	1.81	1.73
3	A	302[B]	EUK	CAP-CLT	3.56	1.82	1.73
2	C	301	NAP	C2A-N3A	3.80	1.38	1.32
3	D	302[A]	EUK	CAO-CLS	3.97	1.83	1.73
2	C	301	NAP	C5A-C4A	4.03	1.49	1.40
2	D	301	NAP	P2B-O2B	4.08	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	C2A-N3A	4.13	1.39	1.32
3	A	302[A]	EUK	CAO-CLS	4.28	1.83	1.73
2	D	301	NAP	C2A-N3A	4.43	1.39	1.32
3	C	302[B]	EUK	CAH-SAK	4.44	1.86	1.76
3	C	302[A]	EUK	CAH-SAK	5.16	1.87	1.76
3	B	302	EUK	CAH-SAK	5.72	1.88	1.76

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	NAP	C4B-O4B-C1B	-6.56	102.99	109.83
2	A	301	NAP	C1B-N9A-C4A	-5.77	116.66	126.64
2	D	301	NAP	C1B-N9A-C4A	-5.33	117.43	126.64
2	C	301	NAP	C1B-N9A-C4A	-4.73	118.46	126.64
2	D	301	NAP	O7N-C7N-C3N	-4.43	114.26	119.62
2	D	301	NAP	N3A-C2A-N1A	-4.40	121.58	128.68
2	B	301	NAP	C1B-N9A-C4A	-4.31	119.19	126.64
2	A	301	NAP	C4B-O4B-C1B	-4.28	105.37	109.83
2	C	301	NAP	C4B-O4B-C1B	-3.72	105.95	109.83
2	B	301	NAP	O7N-C7N-C3N	-3.65	115.20	119.62
3	D	302[B]	EUK	CAE-CAD-SAC	-3.46	107.59	112.00
2	C	301	NAP	O2B-P2B-O1X	-3.42	96.20	109.39
3	A	302[A]	EUK	CAL-CAM-CAR	-3.31	114.31	120.87
2	C	301	NAP	O7N-C7N-C3N	-3.30	115.62	119.62
2	C	301	NAP	N3A-C2A-N1A	-3.09	123.70	128.68
2	B	301	NAP	C5N-C4N-C3N	-3.03	116.71	120.34
2	A	301	NAP	N3A-C2A-N1A	-2.99	123.85	128.68
2	A	301	NAP	O2B-P2B-O1X	-2.82	98.51	109.39
3	C	302[A]	EUK	CAE-CAD-SAC	-2.50	108.82	112.00
2	C	301	NAP	C5N-C6N-N1N	-2.45	116.75	120.39
3	D	302[A]	EUK	CAE-CAD-SAC	-2.38	108.96	112.00
2	B	301	NAP	N3A-C2A-N1A	-2.32	124.94	128.68
3	A	302[B]	EUK	CAE-CAD-SAC	-2.29	109.08	112.00
2	D	301	NAP	O2B-P2B-O1X	-2.27	100.65	109.39
2	A	301	NAP	C5N-C4N-C3N	-2.17	117.74	120.34
3	C	302[A]	EUK	CAL-CAM-CAR	-2.16	116.58	120.87
3	B	302	EUK	CAL-CAM-CAR	-2.12	116.67	120.87
3	B	302	EUK	CAP-CAO-CLS	-2.11	115.60	120.84
3	D	302[A]	EUK	CAL-CAM-CAR	-2.10	116.70	120.87
2	D	301	NAP	C4A-C5A-N7A	-2.10	107.21	109.40
4	C	303	GOL	O2-C2-C1	-2.01	100.25	109.12
3	A	302[A]	EUK	CAE-CAD-SAC	-2.00	109.44	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	NAP	O3X-P2B-O2X	2.01	115.39	107.57
2	D	301	NAP	O2A-PA-O1A	2.03	122.41	112.21
3	D	302[A]	EUK	NAA-CAB-NAF	2.06	125.88	123.22
3	A	302[B]	EUK	CAL-SAK-CAH	2.09	107.27	102.96
3	A	302[B]	EUK	CAO-CAN-CAM	2.12	121.90	120.44
3	A	302[A]	EUK	CAG-CAD-SAC	2.14	128.78	124.84
3	C	302[A]	EUK	NAA-CAB-NAF	2.17	126.01	123.22
2	A	301	NAP	O2X-P2B-O1X	2.18	119.15	110.53
3	A	302[A]	EUK	CAD-CAE-NAF	2.24	113.25	108.04
3	A	302[B]	EUK	NAA-CAB-NAF	2.26	126.12	123.22
3	C	302[B]	EUK	CAN-CAO-CLS	2.27	122.18	118.48
3	D	302[A]	EUK	CAD-CAE-NAF	2.28	113.34	108.04
3	A	302[A]	EUK	CAM-CAL-SAK	2.28	119.51	110.56
3	A	302[B]	EUK	CAG-CAD-SAC	2.31	129.09	124.84
3	D	302[B]	EUK	CAD-CAE-NAF	2.33	113.46	108.04
3	B	302	EUK	CAD-CAE-NAF	2.36	113.53	108.04
2	B	301	NAP	C6N-C5N-C4N	2.36	122.93	119.43
3	D	302[A]	EUK	CAG-CAD-SAC	2.37	129.21	124.84
3	C	302[A]	EUK	CAG-CAD-SAC	2.38	129.23	124.84
2	D	301	NAP	O7N-C7N-N7N	2.40	126.02	122.60
3	C	302[B]	EUK	CAG-CAD-SAC	2.42	129.30	124.84
2	C	301	NAP	N6A-C6A-N1A	2.44	123.64	118.57
3	A	302[B]	EUK	CAD-CAE-NAF	2.50	113.86	108.04
3	C	302[A]	EUK	CAL-CAM-CAN	2.50	124.11	120.38
3	D	302[A]	EUK	CAN-CAO-CLS	2.52	122.58	118.48
3	C	302[A]	EUK	CAD-CAE-NAF	2.56	113.99	108.04
2	C	301	NAP	C2A-N1A-C6A	2.56	123.20	118.77
2	B	301	NAP	C2A-N1A-C6A	2.57	123.22	118.77
2	B	301	NAP	O2A-PA-O1A	2.62	125.34	112.21
4	C	303	GOL	O3-C3-C2	2.65	122.90	110.12
3	B	302	EUK	CAL-CAM-CAN	2.71	124.42	120.38
3	C	302[B]	EUK	CAD-CAE-NAF	2.73	114.39	108.04
2	D	301	NAP	C2A-N1A-C6A	2.85	123.70	118.77
3	B	302	EUK	NAA-CAB-NAF	2.99	127.07	123.22
3	A	302[A]	EUK	CAN-CAO-CLS	3.09	123.50	118.48
3	D	302[A]	EUK	CAL-CAM-CAN	3.19	125.15	120.38
3	B	302	EUK	CAN-CAO-CLS	3.24	123.75	118.48
2	A	301	NAP	C2N-C3N-C4N	3.37	122.13	118.26
3	D	302[B]	EUK	CAG-CAD-SAC	3.41	131.12	124.84
2	B	301	NAP	C3N-C7N-N7N	3.73	121.99	117.75
3	A	302[A]	EUK	CAL-CAM-CAN	4.01	126.37	120.38
2	C	301	NAP	C3N-C7N-N7N	4.75	123.15	117.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302[A]	EUK	1	0
2	B	301	NAP	2	0
3	B	302	EUK	1	0
5	B	304	ACT	1	0
4	B	305	GOL	1	0
3	C	302[A]	EUK	1	0
2	D	301	NAP	1	0
3	D	302[A]	EUK	1	0
3	D	302[B]	EUK	1	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(Å ²)	Q<0.9
1	A	251/288 (87%)	-0.43	1 (0%) 92 93	10, 18, 34, 56	7 (2%)
1	B	252/288 (87%)	-0.47	4 (1%) 72 77	9, 15, 32, 53	1 (0%)
1	C	251/288 (87%)	-0.40	4 (1%) 72 77	11, 18, 38, 60	3 (1%)
1	D	250/288 (86%)	-0.48	1 (0%) 92 93	9, 17, 34, 50	5 (2%)
All	All	1004/1152 (87%)	-0.44	10 (0%) 82 85	9, 17, 34, 60	16 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	ALA	5.5
1	C	113	GLY	4.7
1	C	212	ALA	4.5
1	B	211	VAL	4.2
1	C	221	TRP	2.9
1	B	113	GLY	2.4
1	C	151	SER	2.4
1	D	113	GLY	2.3
1	A	113	GLY	2.2
1	B	151	SER	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	306	6/6	0.76	0.13	39,46,49,51	0
4	GOL	A	303	6/6	0.84	0.11	30,35,40,42	0
4	GOL	C	303	6/6	0.85	0.14	26,36,40,46	0
3	EUK	A	302[B]	20/20	0.91	0.16	18,24,51,56	20
3	EUK	A	302[A]	20/20	0.91	0.16	30,35,46,50	20
3	EUK	C	302[A]	20/20	0.92	0.18	21,24,48,52	20
3	EUK	C	302[B]	20/20	0.92	0.18	29,31,49,51	20
3	EUK	D	302[A]	20/20	0.93	0.15	18,25,42,43	20
3	EUK	D	302[B]	20/20	0.93	0.15	22,29,53,56	20
4	GOL	B	305	6/6	0.94	0.18	28,43,48,53	0
3	EUK	B	302	20/20	0.94	0.12	20,29,65,74	0
2	NAP	C	301	48/48	0.95	0.10	16,20,22,25	0
2	NAP	A	301	48/48	0.96	0.08	15,18,20,22	0
5	ACT	B	303	4/4	0.96	0.06	21,21,22,23	0
5	ACT	B	304	4/4	0.96	0.12	28,28,28,30	0
2	NAP	B	301	48/48	0.97	0.07	12,16,19,21	0
2	NAP	D	301	48/48	0.98	0.06	12,17,20,22	0

6.5 Other polymers

There are no such residues in this entry.