Full wwPDB X-ray Structure Validation Report ⓘ

Dec 14, 2023 – 04:57 am GMT

PDB ID	:	4CM8
Title	:	Crystal structure of pteridine reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor and inhibitor
Authors	:	Barrack, K.L.; Hunter, W.N.
Deposited on	:	2014-01-15
Resolution	:	1.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

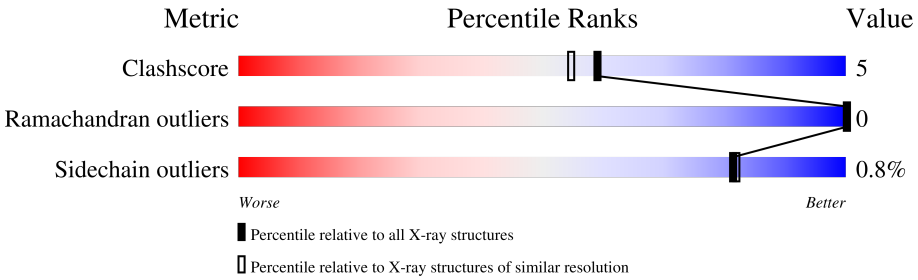
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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
4	IZ9	C	1270	-	-	X	-
4	IZ9	D	1270	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8958 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	5	0
			1888	1189	331	357	11			
1	C	249	Total	C	N	O	S	0	7	0
			1898	1192	335	360	11			
1	D	250	Total	C	N	O	S	0	9	0
			1926	1211	338	365	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	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
C	-19	MET	-	expression tag	UNP O76290
C	-18	GLY	-	expression tag	UNP O76290
C	-17	SER	-	expression tag	UNP O76290

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	expression tag	UNP O76290
D	-18	GLY	-	expression tag	UNP O76290
D	-17	SER	-	expression tag	UNP O76290
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

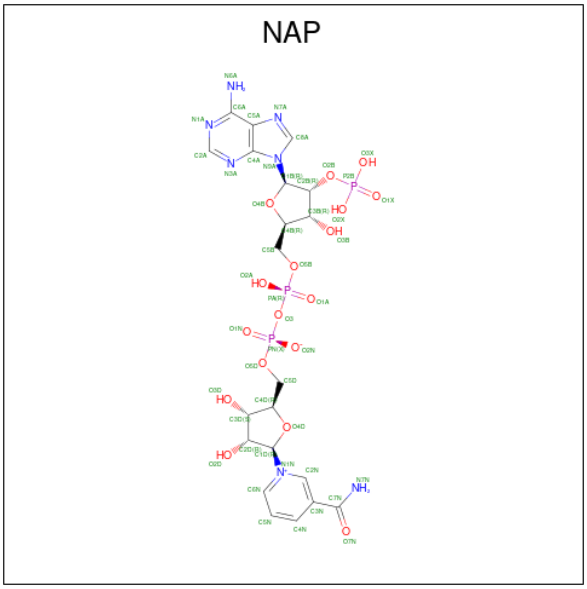
- Molecule 2 is a protein called PTERIDINE REDUCTASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	251	Total	C	N	O	S	0	3	0
			1889	1184	333	361	11			

There are 20 discrepancies between the modelled and reference sequences:

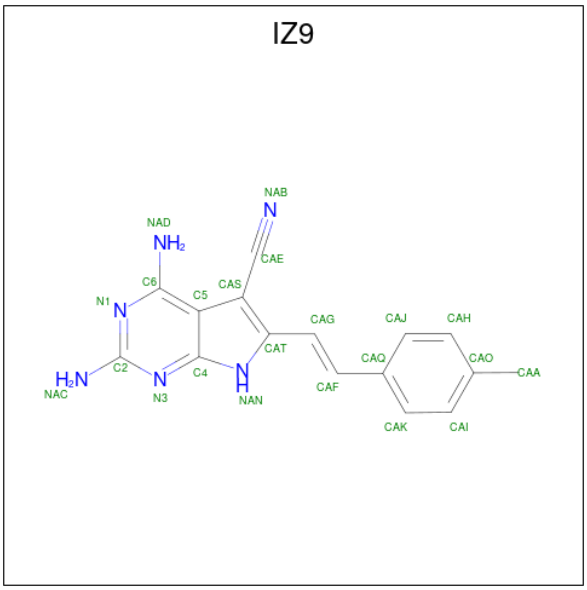
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	expression tag	UNP O76290
B	-18	GLY	-	expression tag	UNP O76290
B	-17	SER	-	expression tag	UNP O76290
B	-16	SER	-	expression tag	UNP O76290
B	-15	HIS	-	expression tag	UNP O76290
B	-14	HIS	-	expression tag	UNP O76290
B	-13	HIS	-	expression tag	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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



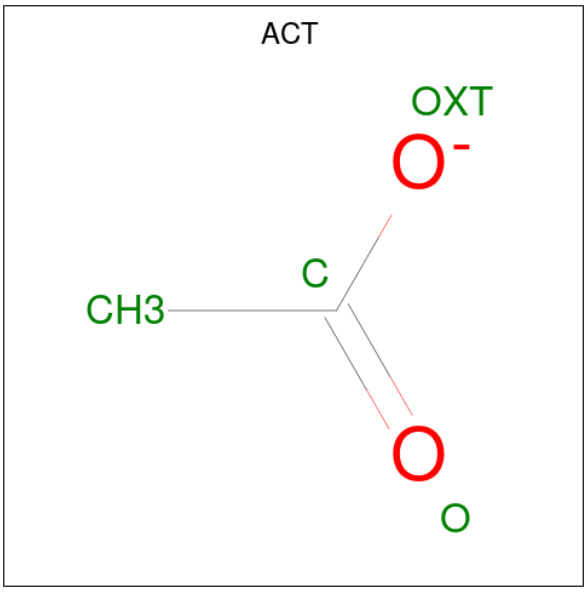
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (E)-2,4-diamino-6-(4-methylstyryl)-7H-pyrrolo[2,3-d]pyrimidine-5-carbonitrile (three-letter code: IZ9) (formula: $C_{16}H_{14}N_6$).



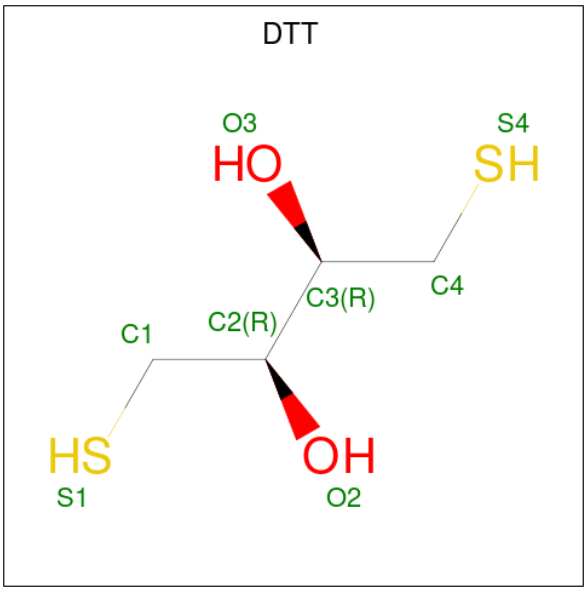
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			22	16	6		
4	B	1	Total	C	N	0	0
			22	16	6		
4	C	1	Total	C	N	0	0
			22	16	6		
4	D	1	Total	C	N	0	0
			22	16	6		

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



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

- Molecule 6 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			8	4	2	2		

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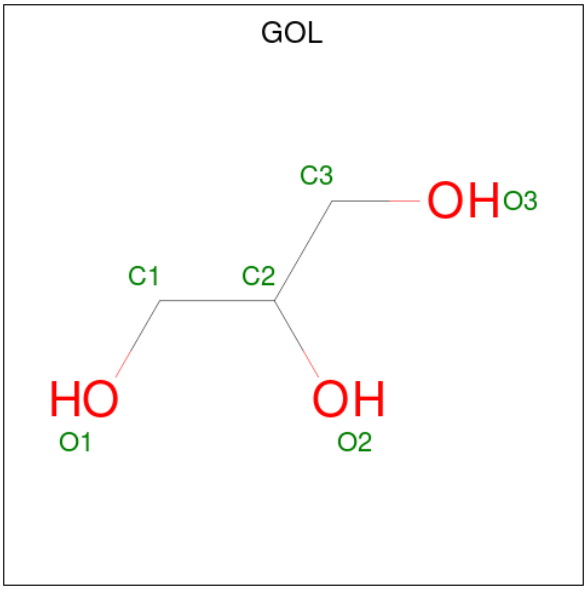
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O S 8 4 2 2	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	303	Total O 303 303	0	0
8	B	290	Total O 290 290	0	0
8	C	242	Total O 242 242	0	0
8	D	206	Total O 206 206	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.60Å 90.00Å 82.60Å 90.00° 115.57° 90.00°	Depositor
Resolution (Å)	15.50 – 1.90	Depositor
% Data completeness (in resolution range)	92.0 (15.50-1.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.141 , 0.192	Depositor
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.109	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
Total number of atoms	8958	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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 26.86 % 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 2.4410e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IZ9, NAP, GOL, DTT, ACT, CSX

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	0.71	0/1919	0.82	4/2603 (0.2%)
1	C	0.72	0/1931	0.79	3/2616 (0.1%)
1	D	0.71	0/1960	0.81	2/2658 (0.1%)
2	B	0.74	0/1919	0.80	0/2603
All	All	0.72	0/7729	0.80	9/10480 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	141	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	82	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	D	222	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	239	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	141	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	141	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	209	LEU	CA-CB-CG	-5.30	103.11	115.30
1	D	141	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	82	ARG	NE-CZ-NH1	5.26	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-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 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	1888	0	1924	15	0
1	C	1898	0	1931	20	0
1	D	1926	0	1961	29	0
2	B	1889	0	1905	13	0
3	A	48	0	25	0	0
3	B	48	0	25	1	0
3	C	48	0	25	0	0
3	D	48	0	25	1	0
4	A	22	0	14	1	0
4	B	22	0	14	0	0
4	C	22	0	14	8	0
4	D	22	0	14	7	0
5	A	4	0	3	0	0
5	C	4	0	3	0	0
6	A	8	0	10	0	0
6	B	8	0	10	1	0
7	C	6	0	8	1	0
7	D	6	0	8	1	0
8	A	303	0	0	7	0
8	B	290	0	0	11	0
8	C	242	0	0	3	0
8	D	206	0	0	7	0
All	All	8958	0	7919	74	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 5.

All (74) 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:C:217:GLU:HG2	8:C:2194:HOH:O	1.52	1.09
2:B:117[B]:GLU:OE1	8:B:2174:HOH:O	1.86	0.94
2:B:211:VAL:O	8:B:2233:HOH:O	1.90	0.89
6:B:1271:DTT:S4	8:B:2290:HOH:O	2.42	0.77
1:D:175[A]:ASN:HB2	8:D:2159:HOH:O	1.84	0.75
1:D:164[B]:VAL:HG22	1:D:179:HIS:CD2	2.22	0.73
8:A:2214:HOH:O	1:C:175[A]:ASN:ND2	2.06	0.71
1:D:168:CSX:HG	4:D:1270:IZ9:CAH	2.04	0.71
1:D:175[B]:ASN:OD1	8:D:2150:HOH:O	2.11	0.68
1:C:168:CSX:HG	4:C:1270:IZ9:CAI	2.09	0.66
2:B:175[A]:ASN:HB2	8:B:2215:HOH:O	1.96	0.66
1:A:168:CSX:HG	4:A:1270:IZ9:CAI	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:GLU:OE1	8:B:2142:HOH:O	2.15	0.64
1:D:62:ASP:OD1	1:D:64[B]:THR:HG23	1.99	0.61
1:C:168:CSX:HG	4:C:1270:IZ9:CAK	2.13	0.61
1:D:168:CSX:HG	4:D:1270:IZ9:CAJ	2.13	0.60
2:B:104:GLN:HG2	1:D:140:GLN:HE22	1.66	0.59
8:B:2168:HOH:O	1:D:140:GLN:NE2	2.27	0.58
1:D:113:GLY:N	8:D:2122:HOH:O	2.36	0.57
8:B:2217:HOH:O	1:D:175[A]:ASN:ND2	2.13	0.57
1:D:210:PRO:HD3	4:D:1270:IZ9:NAB	2.19	0.56
1:C:168:CSX:SG	4:C:1270:IZ9:CAI	2.94	0.56
1:C:75:GLU:OE1	8:C:2117:HOH:O	2.18	0.56
1:D:164[B]:VAL:HG22	1:D:179:HIS:NE2	2.22	0.55
1:A:175[A]:ASN:HB2	8:A:2212:HOH:O	2.06	0.55
1:A:212:ALA:HB3	8:A:2129:HOH:O	2.07	0.53
1:A:175[B]:ASN:HB2	8:A:2212:HOH:O	2.09	0.53
1:A:46:ASP:O	1:A:50:LYS:HD3	2.08	0.53
1:A:65:ASN:HA	1:A:69:LEU:HD22	1.91	0.52
7:C:1272:GOL:H11	8:C:2242:HOH:O	2.09	0.52
1:D:168:CSX:SG	4:D:1270:IZ9:CAH	2.97	0.52
1:D:9:THR:HA	1:D:33:HIS:HB3	1.91	0.52
1:C:138:PHE:O	1:C:142[B]:GLN:HG2	2.10	0.51
1:D:46:ASP:CB	8:D:2059:HOH:O	2.60	0.50
1:A:22:LYS:HG2	1:A:242:ILE:HG12	1.94	0.49
1:A:46:ASP:O	1:A:50:LYS:CD	2.62	0.48
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.48	0.48
1:A:50:LYS:N	1:A:50:LYS:HD2	2.28	0.48
1:A:220:LYS:HD2	8:A:2247:HOH:O	2.14	0.48
2:B:102:LEU:O	1:D:136[B]:MET:HG3	2.14	0.48
1:D:161:ASP:HB3	1:D:164[A]:VAL:HG13	1.96	0.48
1:C:9:THR:HA	1:C:33:HIS:HB3	1.96	0.47
1:A:175[A]:ASN:ND2	8:A:2196:HOH:O	2.20	0.47
2:B:104:GLN:HG2	1:D:140:GLN:NE2	2.30	0.47
1:C:236:GLN:HE21	1:D:250[B]:GLN:CG	2.28	0.47
1:A:267:HIS:CD2	4:D:1270:IZ9:HAA3	2.50	0.47
1:D:46:ASP:HB3	8:D:2059:HOH:O	2.15	0.46
1:C:65:ASN:HA	1:C:69:LEU:HD22	1.99	0.45
1:A:9:THR:HA	1:A:33:HIS:HB3	1.98	0.45
1:C:163:MET:CE	4:C:1270:IZ9:HAA3	2.47	0.45
8:B:2217:HOH:O	1:D:175[B]:ASN:ND2	2.50	0.44
1:D:9:THR:O	1:D:93:ASN:HB3	2.17	0.44
2:B:230:ARG:HD2	8:B:2268:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175[B]:ASN:HB2	8:B:2215:HOH:O	2.18	0.44
1:D:65:ASN:HA	1:D:69:LEU:HD22	1.98	0.44
1:C:46:ASP:O	1:C:50:LYS:HG3	2.17	0.44
1:C:95:SER:CB	4:C:1270:IZ9:HAC2	2.31	0.43
1:D:213:MET:CE	7:D:1271:GOL:H11	2.49	0.43
1:C:221:TRP:HH2	4:C:1270:IZ9:HAA2	1.84	0.43
1:C:221:TRP:CH2	4:C:1270:IZ9:HAA2	2.55	0.42
1:A:17:ARG:HG3	1:A:44:LEU:HD22	2.01	0.41
3:D:1269:NAP:O2A	4:D:1270:IZ9:N1	2.53	0.41
2:B:15:ILE:HB	3:B:1269:NAP:H51N	2.01	0.41
1:C:193:ALA:N	1:C:194:PRO:CD	2.83	0.41
1:C:236:GLN:HE21	1:D:250[B]:GLN:CD	2.23	0.41
8:A:2214:HOH:O	1:C:175[B]:ASN:ND2	2.53	0.41
2:B:98:TYR:HB2	2:B:99:PRO:HD2	2.03	0.41
1:C:210:PRO:HD3	4:C:1270:IZ9:NAB	2.36	0.41
2:B:160:CYS:HB3	8:B:2192:HOH:O	2.20	0.41
1:C:33:HIS:HA	1:C:59:CYS:O	2.21	0.40
1:D:64[B]:THR:HG22	1:D:122:GLU:HG2	2.03	0.40
1:D:175[B]:ASN:HB2	8:D:2159:HOH:O	2.20	0.40
1:D:95:SER:CB	4:D:1270:IZ9:HAC2	2.35	0.40
1:D:220:LYS:CE	8:D:2176:HOH:O	2.69	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	248/288 (86%)	240 (97%)	8 (3%)	0	100	100
1	C	248/288 (86%)	240 (97%)	8 (3%)	0	100	100
1	D	253/288 (88%)	245 (97%)	8 (3%)	0	100	100
2	B	248/288 (86%)	242 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	997/1152 (86%)	967 (97%)	30 (3%)	0	100 100

There are no Ramachandran outliers to report.

4.3.2 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	202/230 (88%)	201 (100%)	1 (0%)	88 89
1	C	204/230 (89%)	203 (100%)	1 (0%)	88 89
1	D	207/230 (90%)	205 (99%)	2 (1%)	76 76
2	B	202/231 (87%)	200 (99%)	2 (1%)	76 76
All	All	815/921 (88%)	809 (99%)	6 (1%)	81 84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
2	B	164	VAL
2	B	166	GLN
1	C	216	GLU
1	D	141	ARG
1	D	151	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	140	GLN

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

14 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.