



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:11 AM GMT

PDB ID : 3BMC
Title : Structure of Pteridine Reductase 1 (PTR1) from Trypanosoma brucei in ternary complex with cofactor (NADP+) and substrate (folate)
Authors : Tulloch, L.B.; Hunter, W.N.
Deposited on : 2007-12-13
Resolution : 2.60 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>

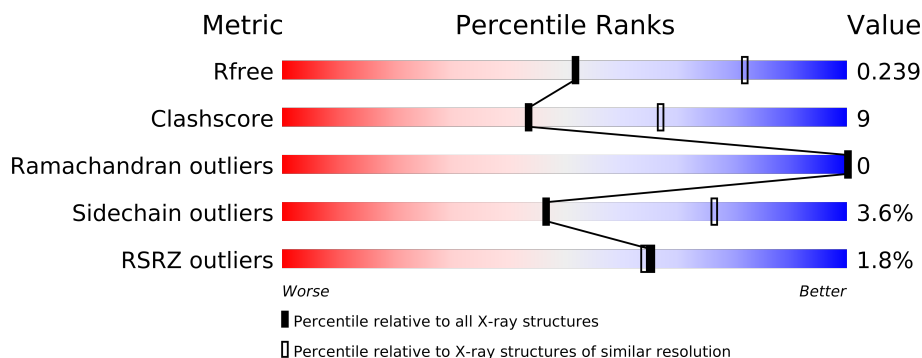
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **FAILED**
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 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	288	
2	B	288	
2	C	288	
2	D	288	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8106 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 Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	6	0
			1877	1184	328	354	11			

There are 20 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

- Molecule 2 is a protein called Pteridine reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	12	0
			1888	1192	329	356	11			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	248	Total	C	N	O	S	0	13	0
			1885	1193	326	355	11			
2	D	249	Total	C	N	O	S	0	10	0
			1883	1186	329	357	11			

There are 60 discrepancies between the modelled and reference sequences:

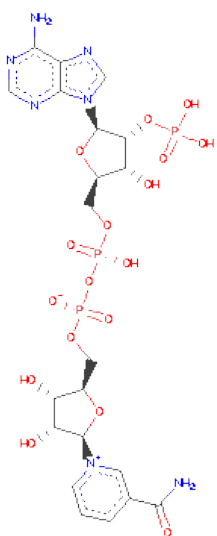
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP O76290
B	-18	GLY	-	EXPRESSION TAG	UNP O76290
B	-17	SER	-	EXPRESSION TAG	UNP O76290
B	-16	SER	-	EXPRESSION TAG	UNP O76290
B	-15	HIS	-	EXPRESSION TAG	UNP O76290
B	-14	HIS	-	EXPRESSION TAG	UNP O76290
B	-13	HIS	-	EXPRESSION TAG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

Continued on next page...

Continued from previous page...

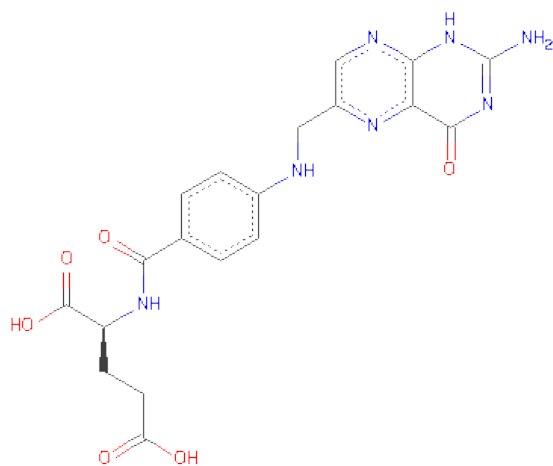
Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	VAL	-	EXPRESSION TAG	UNP O76290
C	-4	PRO	-	EXPRESSION TAG	UNP O76290
C	-3	ARG	-	EXPRESSION TAG	UNP O76290
C	-2	GLY	-	EXPRESSION TAG	UNP O76290
C	-1	SER	-	EXPRESSION TAG	UNP O76290
C	0	HIS	-	EXPRESSION TAG	UNP O76290
D	-19	MET	-	EXPRESSION TAG	UNP O76290
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 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDEPHOSPHATE (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 FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	19	7	6		
4	B	1	Total	C	N	O	0	0
			32	19	7	6		
4	C	1	Total	C	N	O	0	0
			32	19	7	6		
4	D	1	Total	C	N	O	0	0
			32	19	7	6		

- Molecule 5 is water.

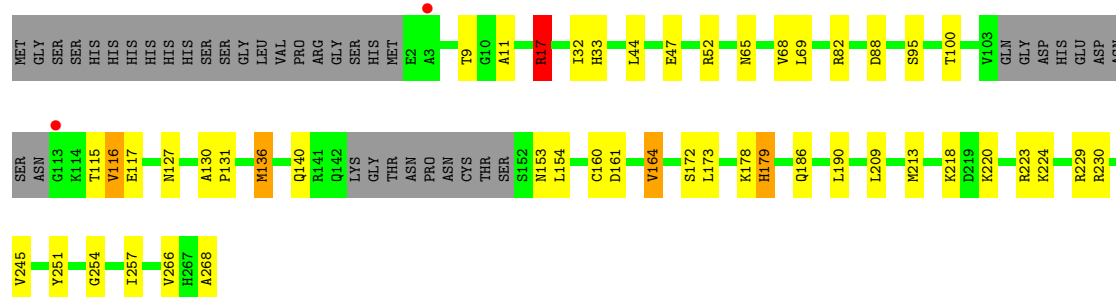
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	80	Total	O	0	0
			80	80		
5	C	55	Total	O	0	0
			55	55		
5	D	51	Total	O	0	0
			51	51		

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.

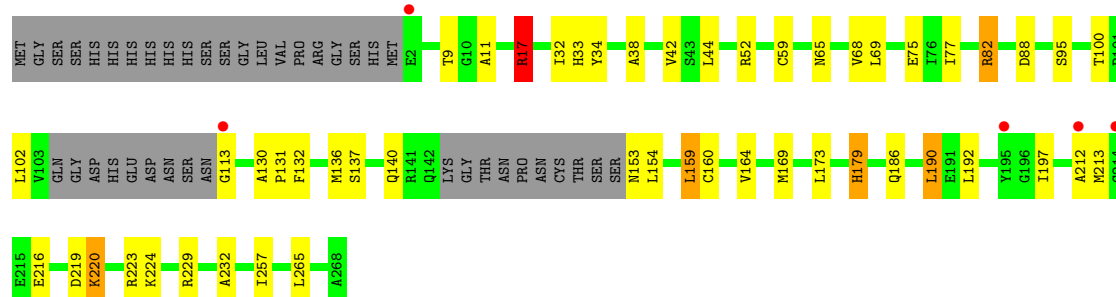
• Molecule 1: Pteridine reductase

Chain A: 



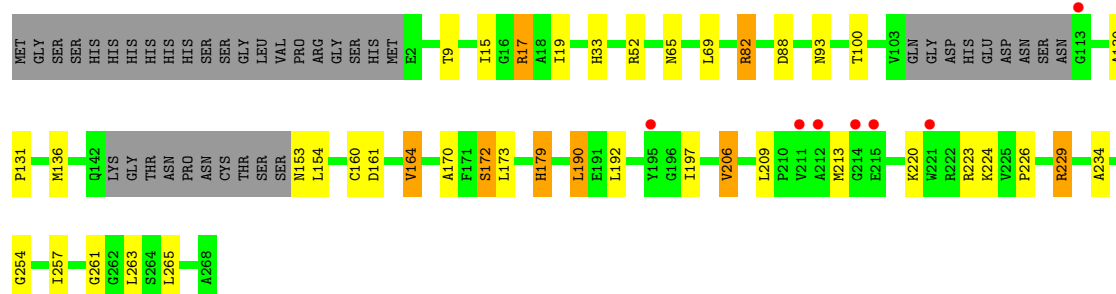
• Molecule 2: Pteridine reductase

Chain B: 



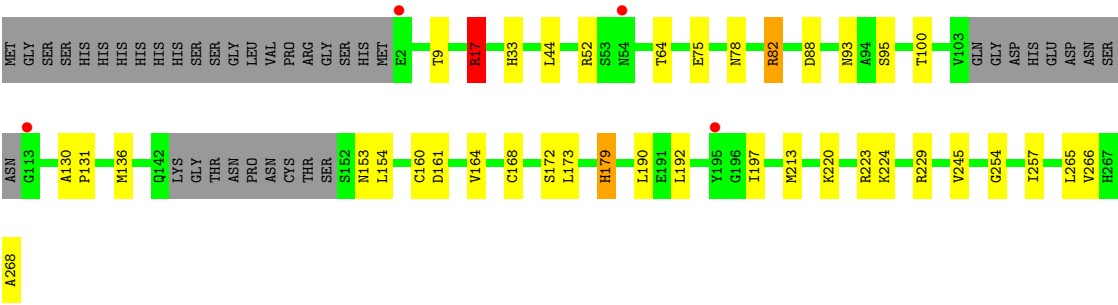
• Molecule 2: Pteridine reductase

Chain C: 



● Molecule 2: Pteridine reductase

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.44Å 88.60Å 81.59Å 90.00° 115.34° 90.00°	Depositor
Resolution (Å)	37.67 – 2.60 37.67 – 2.60	Depositor EDS
% Data completeness (in resolution range)	79.5 (37.67-2.60) 79.5 (37.67-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.189 , 0.244 0.190 , 0.239	Depositor DCC
R_{free} test set	1224 reflections (5.49%)	DCC
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8106	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FOL, NAP, 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	0.47	0/1908	0.80	10/2587 (0.4%)
2	B	0.52	1/1936 (0.1%)	0.80	11/2627 (0.4%)
2	C	0.47	0/1933	0.79	8/2624 (0.3%)
2	D	0.47	0/1925	0.85	9/2612 (0.3%)
All	All	0.48	1/7702 (0.0%)	0.81	38/10450 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	59	CYS	CB-SG	-7.76	1.69	1.82

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	52	ARG	NE-CZ-NH1	-17.14	111.73	120.30
2	C	17	ARG	NE-CZ-NH2	16.00	128.30	120.30
1	A	223	ARG	NE-CZ-NH2	-14.79	112.90	120.30
1	A	223	ARG	NE-CZ-NH1	14.60	127.60	120.30
2	D	52	ARG	NE-CZ-NH2	14.57	127.59	120.30
2	B	82	ARG	NE-CZ-NH1	14.52	127.56	120.30
2	C	17	ARG	NE-CZ-NH1	-13.63	113.48	120.30
2	D	82	ARG	NE-CZ-NH2	-13.40	113.60	120.30
2	B	82	ARG	NE-CZ-NH2	-12.38	114.11	120.30
2	D	82	ARG	NE-CZ-NH1	12.21	126.41	120.30
2	C	82	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	A	82	ARG	NE-CZ-NH1	-9.16	115.72	120.30
2	C	82	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	A	82	ARG	NE-CZ-NH2	8.30	124.45	120.30
2	C	17	ARG	CD-NE-CZ	8.10	134.94	123.60
2	D	52	ARG	CD-NE-CZ	7.71	134.39	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	190	LEU	CA-CB-CG	7.33	132.16	115.30
2	D	17	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	223	ARG	CD-NE-CZ	6.88	133.23	123.60
1	A	17	ARG	NE-CZ-NH1	6.59	123.60	120.30
2	B	159	LEU	CA-CB-CG	-6.58	100.17	115.30
2	B	52	ARG	NE-CZ-NH2	-6.47	117.06	120.30
2	B	17	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	52	ARG	NE-CZ-NH2	-6.33	117.13	120.30
2	B	82	ARG	CD-NE-CZ	6.24	132.33	123.60
1	A	52	ARG	NE-CZ-NH1	5.82	123.21	120.30
2	D	223	ARG	NE-CZ-NH1	-5.81	117.40	120.30
2	D	82	ARG	CD-NE-CZ	5.80	131.72	123.60
2	D	223	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	116	VAL	CB-CA-C	-5.73	100.52	111.40
2	C	223	ARG	NE-CZ-NH1	-5.68	117.46	120.30
2	B	52	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	B	223	ARG	NE-CZ-NH1	-5.60	117.50	120.30
2	C	223	ARG	NE-CZ-NH2	5.36	122.98	120.30
2	B	223	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	82	ARG	CD-NE-CZ	5.12	130.77	123.60
2	C	52	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	B	190	LEU	CB-CG-CD1	5.09	119.65	111.00

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	1877	0	1918	34	0
2	B	1888	0	1932	40	2
2	C	1885	0	1931	42	1
2	D	1883	0	1918	30	0
3	A	48	0	25	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	25	3	0
3	C	48	0	25	2	0
3	D	48	0	25	1	0
4	A	32	0	17	5	0
4	B	32	0	17	6	0
4	C	32	0	17	5	0
4	D	32	0	17	6	0
5	A	67	0	0	4	1
5	B	80	0	0	12	0
5	C	55	0	0	11	0
5	D	51	0	0	5	0
All	All	8106	0	7867	137	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (137) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:206[B]:VAL:CG2	2:C:209[B]:LEU:HD11	1.77	1.14
2:B:212:ALA:HB3	5:B:336:HOH:O	1.57	1.05
2:C:179:HIS:ND1	5:C:336:HOH:O	1.90	1.03
2:C:206[B]:VAL:CG2	2:C:209[B]:LEU:CD1	2.48	0.90
1:A:179:HIS:ND1	5:C:336:HOH:O	2.01	0.82
2:C:206[B]:VAL:HG21	2:C:209[B]:LEU:HD11	1.59	0.82
2:B:220:LYS:HD3	5:B:315:HOH:O	1.80	0.82
2:B:153:ASN:HA	5:B:329:HOH:O	1.81	0.80
2:C:179:HIS:CE1	5:C:336:HOH:O	2.30	0.79
2:B:219:ASP:OD2	5:B:299:HOH:O	2.00	0.79
1:A:179:HIS:CE1	5:C:336:HOH:O	2.35	0.77
2:C:206[B]:VAL:HG23	2:C:209[B]:LEU:CD1	2.16	0.75
1:A:47:GLU:HG3	5:A:316:HOH:O	1.85	0.75
2:D:75:GLU:OE2	5:D:310:HOH:O	2.06	0.74
2:D:213:MET:HE3	4:D:270:FOL:H12	1.71	0.72
2:C:213:MET:HE3	4:C:270:FOL:H12	1.71	0.72
2:B:75:GLU:OE2	2:B:82:ARG:NH2	2.27	0.66
2:C:130:ALA:HB3	2:C:131:PRO:HD3	1.80	0.64
2:D:9:THR:HA	2:D:33:HIS:HB3	1.79	0.63
2:B:113:GLY:N	5:B:325:HOH:O	2.32	0.63
2:D:213:MET:CE	4:D:270:FOL:C12	2.78	0.62
2:C:9:THR:HA	2:C:33:HIS:HB3	1.82	0.61
2:C:213:MET:CE	4:C:270:FOL:C12	2.79	0.61
2:D:164[A]:VAL:HG22	2:D:179:HIS:CD2	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:9:THR:HA	2:B:33:HIS:HB3	1.83	0.61
2:C:206[B]:VAL:HG23	2:C:209[B]:LEU:HD11	1.75	0.60
2:C:229:ARG:HG2	5:C:339:HOH:O	2.00	0.60
2:C:15[B]:ILE:HG23	3:C:269:NAP:H51N	1.85	0.59
1:A:17:ARG:NH2	5:A:305:HOH:O	2.35	0.59
2:B:68:VAL:HG23	5:B:319:HOH:O	2.03	0.59
2:B:164:VAL:HG22	2:B:179:HIS:CD2	2.38	0.59
2:C:17:ARG:CZ	5:C:338:HOH:O	2.51	0.58
1:A:9:THR:HA	1:A:33:HIS:HB3	1.85	0.58
2:B:224:LYS:HE3	5:B:339:HOH:O	2.04	0.58
2:B:213:MET:HE3	4:B:270:FOL:H12	1.87	0.57
2:B:130:ALA:HB3	2:B:131:PRO:HD3	1.86	0.57
2:C:153:ASN:N	5:C:362:HOH:O	2.38	0.57
1:A:213:MET:HE3	4:A:270:FOL:H12	1.87	0.57
4:B:270:FOL:HG1	5:B:331:HOH:O	2.04	0.57
2:D:75:GLU:OE2	2:D:82:ARG:NH2	2.32	0.57
2:D:213:MET:HE1	4:D:270:FOL:C12	2.35	0.57
2:D:213:MET:HE3	4:D:270:FOL:C12	2.36	0.56
2:B:216[B]:GLU:CD	2:B:216[B]:GLU:H	2.09	0.56
2:D:64:THR:O	5:D:332:HOH:O	2.18	0.55
1:A:160:CYS:O	3:A:269:NAP:H6N	2.06	0.55
1:A:186:GLN:NE2	5:A:286:HOH:O	2.23	0.55
2:C:17:ARG:NH2	5:C:338:HOH:O	2.38	0.55
2:C:213:MET:HE3	4:C:270:FOL:C12	2.36	0.55
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.89	0.55
2:D:130:ALA:HB3	2:D:131:PRO:HD3	1.89	0.55
2:C:213:MET:HE1	4:C:270:FOL:C12	2.38	0.54
2:B:38:ALA:O	2:B:42:VAL:HG13	2.08	0.53
2:D:78:ASN:HB3	5:D:339:HOH:O	2.08	0.53
2:B:213:MET:CE	4:B:270:FOL:C12	2.87	0.53
2:D:17:ARG:HH11	2:D:44:LEU:HB2	1.74	0.53
2:C:161:ASP:O	2:C:164:VAL:HG22	2.09	0.52
2:D:88:ASP:HA	2:D:154:LEU:HD23	1.92	0.52
1:A:213:MET:CE	4:A:270:FOL:C12	2.87	0.52
2:B:88:ASP:HA	2:B:154:LEU:HD23	1.91	0.52
1:A:254:GLY:HA3	2:B:265:LEU:HD11	1.91	0.52
2:D:213:MET:CE	4:D:270:FOL:H12	2.38	0.51
2:C:160:CYS:O	3:C:269:NAP:H6N	2.11	0.51
2:C:213:MET:CE	4:C:270:FOL:H12	2.37	0.51
2:B:160:CYS:O	3:B:269:NAP:H6N	2.11	0.51
1:A:100:THR:HG21	1:A:173:LEU:HD12	1.93	0.51
2:B:77[B]:ILE:HD13	2:B:137:SER:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:15[B]:ILE:HD11	2:C:19:ILE:HD11	1.93	0.50
1:A:17:ARG:HH11	1:A:44:LEU:HB2	1.75	0.50
2:B:11:ALA:HB3	2:B:32[A]:ILE:HG23	1.92	0.50
2:C:206[B]:VAL:HG22	2:C:209[B]:LEU:CD1	2.37	0.49
2:C:88:ASP:HA	2:C:154:LEU:HD23	1.93	0.49
2:C:15[B]:ILE:HD13	2:C:93:ASN:OD1	2.13	0.49
2:D:161:ASP:O	2:D:164[B]:VAL:HG22	2.12	0.49
2:D:160:CYS:O	3:D:269:NAP:H6N	2.12	0.49
2:B:32[A]:ILE:HG12	2:B:44:LEU:HD23	1.95	0.48
1:A:88:ASP:HA	1:A:154:LEU:HD23	1.95	0.48
2:B:34[A]:TYR:CE1	2:B:38:ALA:HA	2.49	0.47
2:B:136:MET:O	2:B:140[B]:GLN:HG3	2.14	0.47
3:B:269:NAP:H8A	5:B:338:HOH:O	2.14	0.47
1:A:11:ALA:HB3	1:A:32:ILE:HG23	1.96	0.47
2:B:186:GLN:HB2	5:B:314:HOH:O	2.14	0.47
2:C:100:THR:HG21	2:C:173:LEU:HD12	1.96	0.47
1:A:161:ASP:HB3	1:A:164:VAL:HG13	1.97	0.47
2:C:265:LEU:HD11	2:D:254:GLY:HA3	1.97	0.47
2:B:169:MET:HE1	5:D:311:HOH:O	2.15	0.46
2:C:206[B]:VAL:HG22	2:C:209[B]:LEU:HD11	1.81	0.46
1:A:213:MET:HE3	4:A:270:FOL:C12	2.46	0.46
2:D:168:CYS:SG	4:D:270:FOL:H16	2.55	0.46
2:B:213:MET:HE1	4:B:270:FOL:C12	2.46	0.46
1:A:268:ALA:HB2	2:D:266:VAL:HB	1.96	0.46
1:A:127:ASN:OD1	1:A:178:LYS:HE2	2.15	0.46
2:D:9:THR:O	2:D:93:ASN:HB3	2.14	0.46
1:A:17:ARG:NH1	1:A:44:LEU:HD13	2.30	0.46
2:D:100:THR:HG21	2:D:173:LEU:HD12	1.97	0.46
1:A:213:MET:HE1	4:A:270:FOL:C12	2.47	0.45
2:B:17:ARG:NH1	2:B:44:LEU:HD13	2.32	0.45
1:A:179:HIS:HD1	2:C:179:HIS:HD1	1.65	0.45
2:B:17:ARG:HH11	2:B:44:LEU:HB2	1.82	0.45
2:C:226:PRO:HD2	2:C:261:GLY:O	2.17	0.44
1:A:209[A]:LEU:HD22	1:A:218:LYS:HA	1.99	0.44
2:C:172:SER:OG	5:C:314:HOH:O	2.20	0.44
2:C:65:ASN:HA	2:C:69:LEU:HD22	1.99	0.44
2:B:213:MET:HE3	4:B:270:FOL:C12	2.47	0.44
1:A:136:MET:O	1:A:140:GLN:HG3	2.16	0.43
1:A:266:VAL:HB	2:D:268:ALA:HB2	2.00	0.43
2:D:153:ASN:ND2	2:D:245:VAL:O	2.52	0.43
1:A:230:ARG:HD3	5:A:318:HOH:O	2.17	0.43
2:D:17:ARG:NH1	2:D:44:LEU:HD13	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:ILE:HG12	2:B:257:ILE:HG12	2.00	0.43
2:B:213:MET:CE	4:B:270:FOL:H12	2.47	0.43
2:B:220:LYS:CD	5:B:315:HOH:O	2.51	0.43
1:A:95:SER:HB3	3:A:269:NAP:H3D	2.01	0.42
2:C:170:ALA:HA	5:C:314:HOH:O	2.18	0.42
2:C:15[B]:ILE:HA	2:C:234:ALA:HB1	2.02	0.42
2:C:17:ARG:NH2	5:C:343:HOH:O	2.51	0.42
1:A:213:MET:CE	4:A:270:FOL:H12	2.50	0.42
2:B:95:SER:HB3	3:B:269:NAP:H3D	2.02	0.42
2:C:254:GLY:HA3	2:D:265:LEU:HD11	2.02	0.42
1:A:220:LYS:O	1:A:224:LYS:HG3	2.20	0.42
2:C:192:LEU:HB3	2:C:197:ILE:HB	2.02	0.42
2:C:206[A]:VAL:HG22	2:C:263:LEU:HD22	2.02	0.41
2:C:220:LYS:O	2:C:224:LYS:HG3	2.20	0.41
2:D:220:LYS:O	2:D:224:LYS:HG3	2.20	0.41
2:C:190:LEU:HD12	2:D:265:LEU:HB3	2.02	0.41
2:B:132:PHE:HE1	2:D:172[A]:SER:HG	1.68	0.41
1:A:115:THR:OG1	1:A:117[A]:GLU:HG2	2.19	0.41
2:C:9:THR:O	2:C:93:ASN:HB3	2.21	0.41
2:B:192:LEU:HB3	2:B:197:ILE:HB	2.02	0.41
2:B:102[B]:LEU:HD13	5:D:317:HOH:O	2.20	0.41
2:B:65:ASN:HA	2:B:69:LEU:HD22	2.02	0.41
2:C:257:ILE:HG12	2:D:257:ILE:HG12	2.02	0.41
2:D:192:LEU:HB3	2:D:197:ILE:HB	2.03	0.41
1:A:65:ASN:HA	1:A:69:LEU:HD22	2.02	0.41
1:A:251:TYR:CE2	2:B:232:ALA:HB2	2.56	0.40
1:A:153:ASN:ND2	1:A:245:VAL:O	2.54	0.40
2:B:82:ARG:NE	5:B:317:HOH:O	2.54	0.40
2:B:100:THR:HG21	2:B:173:LEU:HD12	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:82:ARG:NH1	2:C:82:ARG:O[1_454]	1.98	0.22
2:B:216[B]:GLU:OE2	5:A:305:HOH:O[2_555]	1.98	0.22

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	246/288 (85%)	237 (96%)	9 (4%)	0	100	100
2	B	250/288 (87%)	242 (97%)	8 (3%)	0	100	100
2	C	248/288 (86%)	239 (96%)	9 (4%)	0	100	100
2	D	249/288 (86%)	240 (96%)	9 (4%)	0	100	100
All	All	993/1152 (86%)	958 (96%)	35 (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	200/230 (87%)	191 (96%)	9 (4%)	38	67
2	B	204/231 (88%)	198 (97%)	6 (3%)	55	83
2	C	203/231 (88%)	195 (96%)	8 (4%)	43	74
2	D	203/231 (88%)	197 (97%)	6 (3%)	53	82
All	All	810/923 (88%)	781 (96%)	29 (4%)	47	76

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	68	VAL
1	A	116	VAL
1	A	136	MET
1	A	164	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	172	SER
1	A	179	HIS
1	A	190	LEU
1	A	229	ARG
2	B	17	ARG
2	B	159	LEU
2	B	179	HIS
2	B	190	LEU
2	B	220	LYS
2	B	229	ARG
2	C	136	MET
2	C	164	VAL
2	C	172	SER
2	C	179	HIS
2	C	190	LEU
2	C	206[A]	VAL
2	C	206[B]	VAL
2	C	229	ARG
2	D	17	ARG
2	D	95	SER
2	D	136	MET
2	D	179	HIS
2	D	190	LEU
2	D	229	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
2	B	166	GLN
2	B	250	GLN
2	C	166	GLN
2	D	67[A]	ASN
2	D	166	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSX	A	168	1	4,6,7	9.10	1 (25%)	3,6,8	5.18	3 (100%)

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
1	CSX	A	168	1	-	0/2/5/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	CSX	O-C	18.08	1.23	1.11

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	CSX	C-CA-N	-7.26	106.58	113.83
1	A	168	CSX	CA-CB-SG	4.37	116.85	110.82
1	A	168	CSX	CB-CA-N	2.94	115.17	110.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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$
3	NAP	A	269	-	52,52,52	1.41	4 (7%)	80,80,80	1.73	8 (10%)
4	FOL	A	270	-	34,34,34	1.53	3 (8%)	45,47,47	2.64	16 (35%)
3	NAP	B	269	-	52,52,52	1.29	3 (5%)	80,80,80	1.76	8 (10%)
4	FOL	B	270	-	34,34,34	1.66	5 (14%)	45,47,47	2.67	19 (42%)
3	NAP	C	269	-	52,52,52	1.38	4 (7%)	80,80,80	1.79	11 (13%)
4	FOL	C	270	-	34,34,34	1.48	3 (8%)	45,47,47	2.62	17 (37%)
3	NAP	D	269	-	52,52,52	1.31	4 (7%)	80,80,80	1.77	10 (12%)
4	FOL	D	270	-	34,34,34	1.54	3 (8%)	45,47,47	2.65	17 (37%)

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	NAP	A	269	-	-	0/35/67/67	0/3/5/5
4	FOL	A	270	-	-	0/22/22/22	0/1/3/3
3	NAP	B	269	-	-	0/35/67/67	0/3/5/5
4	FOL	B	270	-	-	0/22/22/22	0/1/3/3
3	NAP	C	269	-	-	0/35/67/67	0/3/5/5
4	FOL	C	270	-	-	0/22/22/22	0/1/3/3
3	NAP	D	269	-	-	0/35/67/67	0/3/5/5
4	FOL	D	270	-	-	0/22/22/22	0/1/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	269	NAP	O7N-C7N	7.40	1.41	1.24
3	C	269	NAP	O7N-C7N	7.32	1.41	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	269	NAP	O7N-C7N	7.19	1.41	1.24
3	B	269	NAP	O7N-C7N	6.93	1.40	1.24
4	B	270	FOL	O4-C4	6.53	1.37	1.24
4	D	270	FOL	O4-C4	6.46	1.37	1.24
4	A	270	FOL	O4-C4	6.41	1.37	1.24
4	C	270	FOL	O4-C4	6.12	1.36	1.24
3	C	269	NAP	C2A-N3A	3.15	1.38	1.32
3	A	269	NAP	C2A-N3A	3.08	1.38	1.32
3	D	269	NAP	C2A-N3A	2.98	1.38	1.32
3	B	269	NAP	C2A-N3A	2.98	1.38	1.32
4	B	270	FOL	C6-N5	2.86	1.38	1.32
4	B	270	FOL	C2-N3	2.85	1.37	1.33
3	A	269	NAP	C2N-N1N	2.84	1.38	1.35
3	A	269	NAP	C2A-N1A	2.70	1.39	1.33
3	C	269	NAP	C2N-N1N	2.60	1.38	1.35
4	B	270	FOL	C8A-N1	-2.57	1.34	1.37
4	A	270	FOL	C6-N5	2.52	1.38	1.32
4	B	270	FOL	C2-NA2	2.51	1.36	1.32
3	B	269	NAP	C2A-N1A	2.48	1.38	1.33
3	C	269	NAP	C2A-N1A	2.47	1.38	1.33
4	D	270	FOL	C6-N5	2.36	1.37	1.32
3	D	269	NAP	C2N-N1N	2.28	1.38	1.35
4	C	270	FOL	C6-N5	2.27	1.37	1.32
3	D	269	NAP	C2A-N1A	2.25	1.38	1.33
4	C	270	FOL	C2-NA2	2.21	1.35	1.32
4	A	270	FOL	C8A-N1	-2.15	1.35	1.37
4	D	270	FOL	C2-NA2	2.01	1.35	1.32

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	269	NAP	N3A-C2A-N1A	-10.69	119.78	128.71
3	B	269	NAP	N3A-C2A-N1A	-10.27	120.12	128.71
4	A	270	FOL	C6-C9-N10	-10.15	89.86	113.33
4	D	270	FOL	C6-C9-N10	-10.06	90.08	113.33
4	B	270	FOL	C6-C9-N10	-9.96	90.29	113.33
3	D	269	NAP	N3A-C2A-N1A	-9.63	120.66	128.71
4	C	270	FOL	C6-C9-N10	-9.52	91.31	113.33
3	A	269	NAP	N3A-C2A-N1A	-9.40	120.85	128.71
3	A	269	NAP	O4B-C1B-N9A	6.82	114.78	108.44
3	B	269	NAP	O4B-C1B-N9A	6.75	114.72	108.44
3	D	269	NAP	O4B-C1B-N9A	6.67	114.65	108.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	269	NAP	O4B-C1B-N9A	6.09	114.11	108.44
4	A	270	FOL	C13-C14-N10	-5.61	109.56	121.02
4	D	270	FOL	C13-C14-N10	-5.57	109.65	121.02
4	C	270	FOL	C13-C14-N10	-5.48	109.83	121.02
4	B	270	FOL	C13-C14-N10	-5.34	110.12	121.02
3	D	269	NAP	O4D-C1D-N1N	4.76	112.82	107.95
4	C	270	FOL	CB-CA-N	-4.65	101.96	110.83
4	C	270	FOL	C11-C-N	-4.57	109.28	116.89
4	C	270	FOL	C4-N3-C2	4.50	121.78	116.91
4	D	270	FOL	CB-CA-N	-4.50	102.27	110.83
4	B	270	FOL	CB-CA-N	-4.48	102.29	110.83
4	A	270	FOL	C11-C-N	-4.36	109.63	116.89
4	B	270	FOL	C11-C-N	-4.34	109.67	116.89
3	C	269	NAP	O4D-C1D-N1N	4.26	112.31	107.95
4	D	270	FOL	C11-C-N	-4.17	109.94	116.89
4	D	270	FOL	C4-N3-C2	4.03	121.26	116.91
4	D	270	FOL	C15-C14-N10	3.93	129.05	121.02
4	A	270	FOL	CB-CA-N	-3.93	103.35	110.83
3	B	269	NAP	O4D-C1D-N1N	3.92	111.96	107.95
4	A	270	FOL	C15-C14-N10	3.89	128.95	121.02
4	A	270	FOL	C4-N3-C2	3.87	121.09	116.91
3	A	269	NAP	O4D-C1D-N1N	3.80	111.83	107.95
4	C	270	FOL	C15-C14-N10	3.74	128.66	121.02
4	B	270	FOL	C15-C14-N10	3.62	128.41	121.02
4	C	270	FOL	CA-N-C	3.58	129.79	121.80
4	B	270	FOL	C7-C6-N5	-3.50	118.30	120.75
4	B	270	FOL	C9-N10-C14	3.47	131.77	122.29
4	D	270	FOL	C9-N10-C14	3.46	131.74	122.29
4	C	270	FOL	C9-N10-C14	3.42	131.62	122.29
4	B	270	FOL	CA-N-C	3.35	129.28	121.80
4	D	270	FOL	CA-N-C	3.33	129.24	121.80
4	B	270	FOL	C7-N8-C8A	3.32	121.34	116.62
4	A	270	FOL	C12-C11-C	-3.28	110.39	120.56
3	D	269	NAP	N3A-C4A-N9A	3.20	131.21	125.43
4	D	270	FOL	C12-C11-C	-3.19	110.68	120.56
3	D	269	NAP	C2D-C1D-N1N	-3.17	108.49	113.86
3	A	269	NAP	C2D-C1D-N1N	-3.13	108.56	113.86
4	A	270	FOL	C9-N10-C14	3.09	130.72	122.29
4	B	270	FOL	C12-C11-C	-3.03	111.17	120.56
3	C	269	NAP	N3A-C4A-N9A	3.03	130.90	125.43
3	A	269	NAP	N3A-C4A-N9A	3.02	130.88	125.43
3	D	269	NAP	C4B-O4B-C1B	-3.00	106.49	109.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	269	NAP	C3N-C7N-N7N	2.99	121.18	117.77
4	A	270	FOL	NA2-C2-N1	2.96	121.12	117.86
3	B	269	NAP	N3A-C4A-N9A	2.96	130.78	125.43
4	B	270	FOL	C4-N3-C2	2.94	120.08	116.91
4	C	270	FOL	C12-C11-C	-2.86	111.70	120.56
4	A	270	FOL	CB-CG-CD	-2.81	106.06	112.88
3	C	269	NAP	C2D-C1D-N1N	-2.79	109.14	113.86
4	D	270	FOL	C16-C11-C	2.76	129.12	120.56
4	B	270	FOL	CB-CA-CT	-2.70	104.89	110.71
4	A	270	FOL	C16-C11-C	2.68	128.87	120.56
4	A	270	FOL	C7-N8-C8A	2.67	120.42	116.62
4	A	270	FOL	CA-N-C	2.65	127.71	121.80
4	B	270	FOL	C16-C11-C	2.61	128.67	120.56
4	D	270	FOL	C7-N8-C8A	2.56	120.26	116.62
4	C	270	FOL	O-C-N	2.55	127.04	122.44
4	D	270	FOL	C4-C4A-N5	2.54	123.96	119.75
3	A	269	NAP	C4A-C5A-N7A	-2.52	107.37	109.52
4	B	270	FOL	O-C-N	2.49	126.94	122.44
3	B	269	NAP	C2D-C1D-N1N	-2.49	109.64	113.86
4	A	270	FOL	C6-C7-N8	-2.49	120.54	123.16
4	B	270	FOL	C9-C6-N5	2.47	121.34	116.79
4	C	270	FOL	C16-C11-C	2.44	128.13	120.56
4	B	270	FOL	C4-C4A-N5	2.44	123.79	119.75
4	D	270	FOL	C7-C6-N5	-2.39	119.08	120.75
4	B	270	FOL	C6-C7-N8	-2.37	120.67	123.16
4	D	270	FOL	CB-CA-CT	-2.33	105.69	110.71
4	B	270	FOL	CB-CG-CD	-2.33	107.24	112.88
3	B	269	NAP	C4B-O4B-C1B	-2.32	107.23	109.75
3	C	269	NAP	C4B-O4B-C1B	-2.31	107.24	109.75
4	C	270	FOL	CB-CG-CD	-2.29	107.31	112.88
4	C	270	FOL	C7-C6-N5	-2.26	119.17	120.75
4	C	270	FOL	C4-C4A-N5	2.24	123.45	119.75
4	D	270	FOL	CB-CG-CD	-2.24	107.45	112.88
4	C	270	FOL	C7-N8-C8A	2.23	119.79	116.62
3	C	269	NAP	C3N-C7N-N7N	2.20	120.28	117.77
3	A	269	NAP	N7A-C8A-N9A	-2.20	108.14	114.36
4	D	270	FOL	C15-C16-C11	-2.19	118.14	120.76
4	B	270	FOL	C4A-C8A-N8	-2.18	120.09	123.01
3	D	269	NAP	C3N-C7N-N7N	2.14	120.20	117.77
3	D	269	NAP	C4A-C5A-N7A	-2.13	107.70	109.52
3	B	269	NAP	O7N-C7N-C3N	-2.12	117.19	119.58
3	C	269	NAP	C4A-C5A-N7A	-2.10	107.73	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	270	FOL	C9-C6-N5	2.09	120.65	116.79
3	D	269	NAP	N7A-C8A-N9A	-2.08	108.48	114.36
4	C	270	FOL	CB-CA-CT	-2.06	106.28	110.71
3	D	269	NAP	C5A-C4A-N3A	-2.06	121.22	125.70
3	C	269	NAP	C1B-N9A-C4A	-2.05	123.09	126.64
4	A	270	FOL	C15-C16-C11	-2.05	118.31	120.76
3	C	269	NAP	C2A-N3A-C4A	2.05	119.84	114.01
3	C	269	NAP	O7N-C7N-N7N	-2.05	119.64	122.59
4	A	270	FOL	C4A-C8A-N8	-2.03	120.29	123.01
3	A	269	NAP	C5A-C4A-N3A	-2.02	121.31	125.70
4	C	270	FOL	NA2-C2-N1	2.01	120.07	117.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	249/288 (86%)	-0.15	2 (0%) 83 85	28, 31, 32, 37	6 (2%)
2	B	248/288 (86%)	-0.20	5 (2%) 62 60	22, 31, 32, 35	2 (0%)
2	C	248/288 (86%)	-0.19	7 (2%) 50 48	28, 31, 32, 36	2 (0%)
2	D	249/288 (86%)	-0.10	4 (1%) 68 69	27, 31, 32, 37	4 (1%)
All	All	994/1152 (86%)	-0.16	18 (1%) 65 64	22, 31, 32, 37	14 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	212	ALA	4.1
2	D	2	GLU	3.3
1	A	113	GLY	3.2
2	C	113	GLY	3.2
2	B	113	GLY	3.0
2	B	214	GLY	2.9
2	C	214	GLY	2.9
2	B	212	ALA	2.9
2	C	215	GLU	2.9
1	A	3	ALA	2.8
2	D	113	GLY	2.4
2	C	211	VAL	2.4
2	C	195	TYR	2.3
2	B	195	TYR	2.3
2	D	195	TYR	2.0
2	C	221	TRP	2.0
2	D	54	ASN	2.0
2	B	2	GLU	2.0

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

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
1	CSX	A	168	7/8	0.12	-0.86	28,31,31,39	0

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
4	FOL	D	270	32/32	0.18	0.37	29,31,32,33	0
4	FOL	C	270	32/32	0.23	0.33	29,31,32,33	0
4	FOL	A	270	32/32	0.18	0.26	29,31,32,33	0
4	FOL	B	270	32/32	0.20	0.21	29,31,32,33	0
3	NAP	A	269	48/48	0.13	-0.28	29,30,31,32	0
3	NAP	C	269	48/48	0.12	-0.74	29,30,31,32	0
3	NAP	D	269	48/48	0.11	-0.84	29,30,31,32	0
3	NAP	B	269	48/48	0.11	-0.97	29,30,31,32	0

6.5 Other polymers

There are no such residues in this entry.