



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 AM GMT

PDB ID : 2C7V
Title : STRUCTURE OF TRYPANOSOMA BRUCEI PTERIDINE REDUCTASE (PTR1) IN TERNARY COMPLEX WITH COFACTOR AND THE ANTIFOLATE METHOTREXATE
Authors : Dawson, A.; Gibellini, F.; Sienkiewicz, N.; Fyfe, P.K.; Mcliskey, K.; Fairlamb, A.H.; Hunter, W.N.
Deposited on : 2005-11-29
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

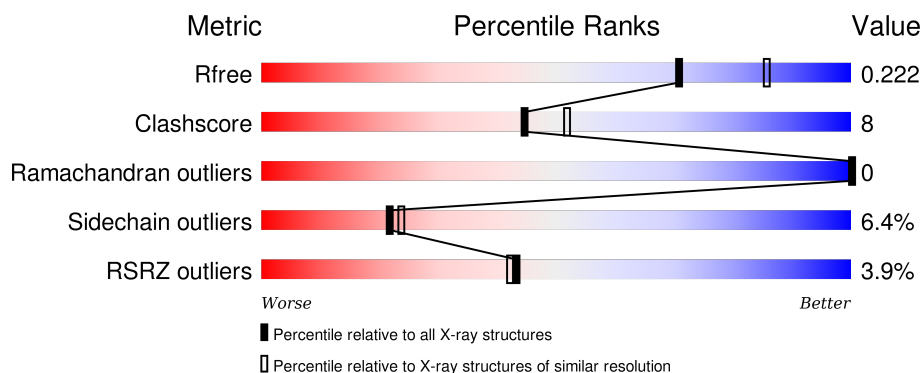
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	268	<div> <div>3%</div> <div>77%</div> <div>15%</div> <div>6%</div> </div>
1	B	268	<div> <div>3%</div> <div>76%</div> <div>15%</div> <div>5%</div> </div>
1	C	268	<div> <div>4%</div> <div>82%</div> <div>13%</div> <div>.</div> </div>
1	D	268	<div> <div>5%</div> <div>79%</div> <div>15%</div> <div>.</div> </div>

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
5	ACT	A	1274	-	-	X	-
5	ACT	B	1274	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8945 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	253	Total	As	C	N	O	S	0	7	0
			1933	2	1215	341	364	11			
1	B	254	Total	As	C	N	O	S	0	7	0
			1945	2	1220	342	370	11			
1	C	260	Total	As	C	N	O	S	0	7	0
			1984	2	1242	352	376	12			
1	D	257	Total	As	C	N	O	S	0	6	0
			1950	2	1225	342	370	11			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



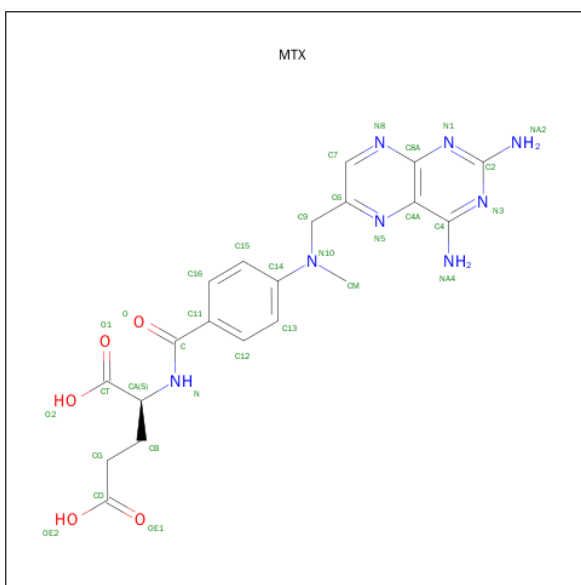
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 33	C 20	N 8	O 5	0	0
3	B	1	Total 33	C 20	N 8	O 5	0	0
3	C	1	Total 33	C 20	N 8	O 5	0	0
3	D	1	Total 33	C 20	N 8	O 5	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ni 1 1	0	0
4	A	1	Total Ni 1 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

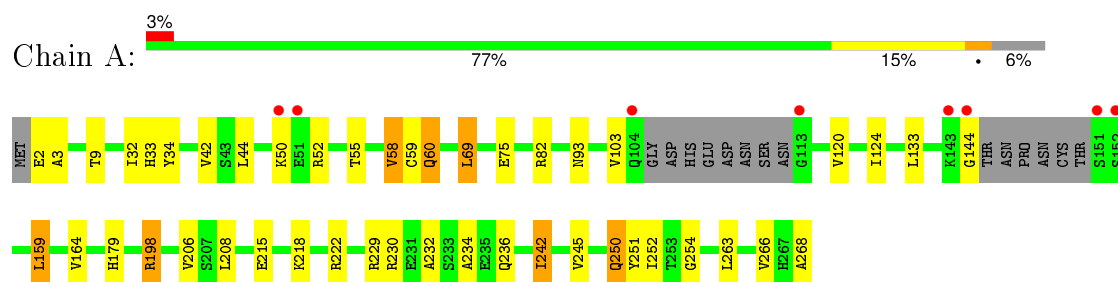
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	203	Total	O	0	0
			203	203		
6	B	217	Total	O	0	0
			217	217		
6	C	192	Total	O	0	0
			192	192		
6	D	187	Total	O	0	0
			187	187		

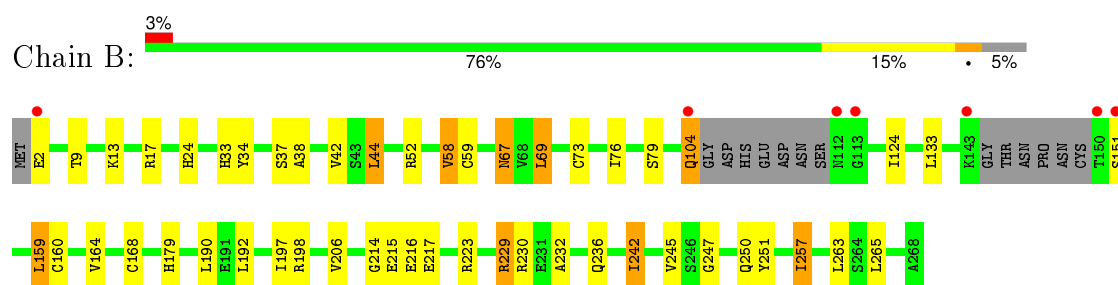
3 Residue-property plots [i](#)

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.

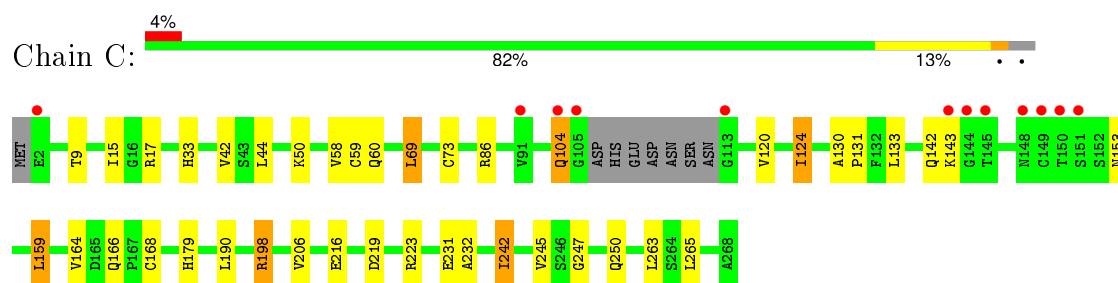
• Molecule 1: PTERIDINE REDUCTASE



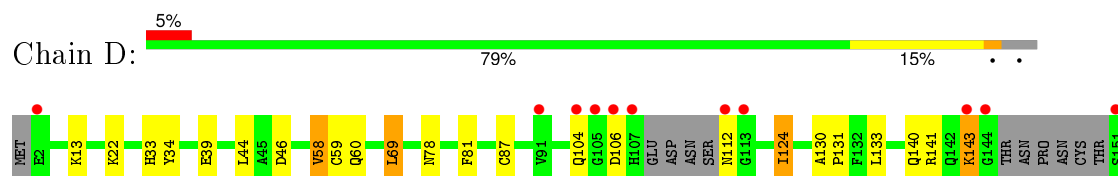
• Molecule 1: PTERIDINE REDUCTASE



• Molecule 1: PTERIDINE REDUCTASE



• Molecule 1: PTERIDINE REDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.66 Å 90.24 Å 82.84 Å 90.00° 115.76° 90.00°	Depositor
Resolution (Å)	74.54 – 2.20 28.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.54-2.20) 99.2 (28.76-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.20 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.153 , 0.223 0.154 , 0.222	Depositor DCC
R_{free} test set	2534 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.7	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	3 of 49904 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8945	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 17.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAF, NI, MTX, NAP, 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	0.50	0/1957	0.64	2/2648 (0.1%)
1	B	0.49	0/1968	0.62	2/2665 (0.1%)
1	C	0.49	0/2009	0.64	3/2722 (0.1%)
1	D	0.49	0/1974	0.66	2/2672 (0.1%)
All	All	0.49	0/7908	0.64	9/10707 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	159	LEU	CA-CB-CG	-7.47	98.12	115.30
1	C	159	LEU	CA-CB-CG	-6.67	99.95	115.30
1	D	198	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	159	LEU	CA-CB-CG	-6.60	100.12	115.30
1	C	198	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	198	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	159	LEU	CA-CB-CG	-5.71	102.17	115.30
1	C	198	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	198	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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	1933	0	1967	40	0
1	B	1945	0	1968	44	0
1	C	1984	0	2009	31	0
1	D	1950	0	1975	32	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	0	0
3	A	33	0	20	0	0
3	B	33	0	20	3	0
3	C	33	0	20	1	0
3	D	33	0	20	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	3	5	0
5	B	4	0	3	5	0
6	A	203	0	0	5	0
6	B	217	0	0	7	0
6	C	192	0	0	3	0
6	D	187	0	0	4	0
All	All	8945	0	8105	128	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 8.

All (128) 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:222:ARG:HH22	5:A:1274:ACT:H3	1.17	1.06
1:B:168:CAF:CE2	3:B:1272:MTX:H15	1.91	0.98
1:B:168:CAF:CE2	3:B:1272:MTX:C15	2.42	0.97
1:B:52:ARG:NH1	6:B:2055:HOH:O	2.10	0.85
1:D:143:LYS:HG2	6:D:2069:HOH:O	1.83	0.78
1:A:120:VAL:O	1:A:124[B]:ILE:HG23	1.84	0.77
1:C:120:VAL:O	1:C:124[A]:ILE:HG23	1.87	0.74
1:C:198:ARG:HD3	6:C:2114:HOH:O	1.87	0.74
1:D:81:PHE:CE2	1:D:143:LYS:HE3	2.23	0.73
1:A:250[A]:GLN:HG3	1:B:236:GLN:HE21	1.53	0.71
1:A:69:LEU:HD13	1:A:133:LEU:HD12	1.73	0.70
1:C:164:VAL:HG22	1:C:179:HIS:CD2	2.27	0.70
1:D:34:TYR:HE2	1:D:58:VAL:HG13	1.56	0.69
1:A:59:CAF:CE2	1:A:75:GLU:HG3	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124[A]:ILE:HG21	1:C:124[A]:ILE:HD11	1.74	0.68
1:D:59:CAF:CE1	1:D:59:CAF:HA	2.24	0.67
1:B:215:GLU:HG2	5:B:1274:ACT:H3	1.77	0.67
1:B:69:LEU:HD13	1:B:133:LEU:HD12	1.77	0.67
1:A:250[A]:GLN:HG3	1:B:236:GLN:NE2	2.10	0.66
1:D:81:PHE:HE2	1:D:143:LYS:HE3	1.60	0.66
1:B:164:VAL:HG22	1:B:179:HIS:CD2	2.33	0.64
1:D:22:LYS:HE2	1:D:239:ASP:OD1	1.99	0.63
1:B:59:CAF:CE1	1:B:59:CAF:HA	2.30	0.62
1:A:52:ARG:NH1	6:A:2049:HOH:O	2.33	0.61
1:B:34:TYR:HE2	1:B:58:VAL:HG13	1.65	0.60
1:C:69:LEU:HD13	1:C:133:LEU:HD12	1.83	0.60
1:D:78[A]:ASN:OD1	1:D:141:ARG:NH1	2.35	0.59
1:B:214:GLY:HA2	5:B:1274:ACT:H1	1.84	0.59
1:A:124[A]:ILE:HG21	1:C:124[A]:ILE:CD1	2.32	0.59
1:A:103:VAL:HG11	1:C:143:LYS:HD3	1.84	0.59
1:D:222:ARG:HD3	1:D:231:GLU:OE2	2.02	0.58
1:C:219:ASP:O	1:C:223[A]:ARG:HG3	2.04	0.58
1:C:104[B]:GLN:HE21	1:C:104[B]:GLN:HA	1.69	0.57
1:A:222:ARG:HH22	5:A:1274:ACT:CH3	2.06	0.57
1:A:198:ARG:HD3	6:A:2111:HOH:O	2.03	0.57
1:D:87:CYS:H	1:D:143:LYS:HZ1	1.53	0.56
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.86	0.56
1:C:59:CAF:CE1	1:C:60:GLN:H	2.18	0.55
1:A:144:GLY:HA3	6:A:2100:HOH:O	2.07	0.55
1:A:222:ARG:NH2	5:A:1274:ACT:H3	2.02	0.55
1:D:112:ASN:HB2	6:D:2079:HOH:O	2.06	0.54
1:A:206:VAL:HG23	1:A:263:LEU:HD22	1.88	0.54
1:B:215:GLU:H	5:B:1274:ACT:H3	1.73	0.53
1:B:24:HIS:O	1:B:52:ARG:NH2	2.39	0.53
1:B:67[A]:ASN:ND2	6:B:2074:HOH:O	2.38	0.53
1:C:9:THR:HA	1:C:33:HIS:HB3	1.91	0.53
1:C:69:LEU:HD22	1:C:73:CYS:SG	2.49	0.53
1:B:223[B]:ARG:NH1	6:B:2169:HOH:O	2.42	0.53
1:A:232:ALA:HB2	1:B:251:TYR:CE2	2.44	0.52
1:C:142:GLN:NE2	6:C:2106:HOH:O	2.37	0.52
1:C:17:ARG:NH2	6:C:2010:HOH:O	2.43	0.52
1:A:230[B]:ARG:NH2	6:A:2156:HOH:O	2.37	0.51
1:B:9:THR:HA	1:B:33:HIS:HB3	1.93	0.51
1:B:215:GLU:H	5:B:1274:ACT:CH3	2.24	0.51
1:A:254:GLY:HA3	1:B:265:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250[A]:GLN:HG3	1:D:236:GLN:HE21	1.76	0.50
1:A:2:GLU:HG2	1:A:3:ALA:N	2.26	0.50
1:B:67[A]:ASN:H	1:B:67[A]:ASN:HD22	1.60	0.50
1:B:216[A]:GLU:HG2	6:B:2161:HOH:O	2.12	0.49
1:C:124[A]:ILE:HG13	1:C:124[A]:ILE:O	2.13	0.49
1:B:17:ARG:HG3	1:B:44:LEU:HG	1.94	0.49
1:A:34:TYR:HE2	1:A:58:VAL:HG13	1.77	0.49
1:B:206:VAL:HG23	1:B:263:LEU:HD22	1.95	0.48
1:A:252:ILE:HD13	1:B:257[A]:ILE:HD11	1.96	0.48
1:B:38:ALA:O	1:B:42:VAL:HG13	2.13	0.48
1:C:120:VAL:HG13	1:C:124[B]:ILE:HD12	1.96	0.47
1:A:164:VAL:HG22	1:A:179:HIS:CD2	2.49	0.47
1:C:206:VAL:HG23	1:C:263:LEU:HD22	1.96	0.47
1:A:34:TYR:CZ	1:A:60:GLN:HB3	2.50	0.47
1:C:232:ALA:HB2	1:D:251:TYR:CE2	2.49	0.47
1:D:164:VAL:HG22	1:D:179:HIS:CD2	2.49	0.47
1:A:52:ARG:NH1	1:A:55:THR:HG21	2.30	0.47
1:A:250[A]:GLN:CG	1:B:236:GLN:HE21	2.24	0.47
1:D:206:VAL:HG23	1:D:263:LEU:HD22	1.96	0.47
1:B:13:LYS:HE2	1:B:37:SER:OG	2.14	0.47
1:D:143:LYS:HD2	1:D:143:LYS:H	1.80	0.46
1:B:34:TYR:CE2	1:B:58:VAL:HG13	2.50	0.46
1:C:265:LEU:O	1:D:190:LEU:HD11	2.15	0.46
1:D:69:LEU:HD13	1:D:133:LEU:HD12	1.97	0.46
1:C:247:GLY:O	1:C:250[B]:GLN:HG2	2.15	0.46
1:D:104:GLN:HE21	1:D:106:ASP:H	1.64	0.45
3:C:1272:MTX:HM1	3:C:1272:MTX:H15	1.82	0.45
1:D:198:ARG:HD3	6:D:2097:HOH:O	2.17	0.45
1:B:104:GLN:HE21	1:B:104:GLN:HA	1.81	0.45
1:D:59:CAF:CE1	1:D:60:GLN:H	2.30	0.45
1:B:59:CAF:CE2	1:B:79:SER:HB2	2.47	0.45
1:B:242:ILE:HA	1:B:245:VAL:HG22	1.99	0.45
1:C:250[A]:GLN:CD	1:D:236:GLN:HE21	2.20	0.45
1:B:247:GLY:O	1:B:250[B]:GLN:HG2	2.18	0.45
1:B:124:ILE:HG21	1:D:124[A]:ILE:CD1	2.46	0.44
1:A:215:GLU:OE1	5:A:1274:ACT:H2	2.17	0.44
1:A:208:LEU:HD11	1:A:234:ALA:HB2	1.98	0.44
1:B:59:CAF:CE1	6:B:2061:HOH:O	2.66	0.44
1:A:251:TYR:CE2	1:B:232:ALA:HB2	2.52	0.44
1:D:143:LYS:HA	6:D:2094:HOH:O	2.16	0.44
1:A:33:HIS:HA	1:A:59:CAF:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:THR:O	1:A:93:ASN:HB3	2.16	0.44
1:A:9:THR:HA	1:A:33:HIS:HB3	1.98	0.44
1:A:59:CAF:CE1	1:A:59:CAF:HA	2.48	0.43
1:C:250[B]:GLN:HA	1:C:250[B]:GLN:HE21	1.83	0.43
1:A:268:ALA:HB2	1:D:266:VAL:HB	2.01	0.43
1:B:151:SER:HA	6:B:2120:HOH:O	2.18	0.43
1:A:242:ILE:HA	1:A:245:VAL:HG22	2.01	0.43
1:A:75:GLU:OE2	1:A:82:ARG:NH2	2.45	0.42
1:D:33:HIS:HA	1:D:59:CAF:O	2.19	0.42
1:B:76:ILE:O	1:B:79:SER:HB3	2.20	0.42
1:C:130:ALA:HB3	1:C:131:PRO:HD3	2.02	0.42
1:C:168:CAF:CE1	1:C:168:CAF:H	2.33	0.42
1:B:223[B]:ARG:HA	1:B:229:ARG:HG3	2.02	0.41
1:C:232:ALA:HB2	1:D:251:TYR:CD2	2.56	0.41
1:A:266:VAL:HB	1:D:268:ALA:HB2	2.02	0.41
1:C:265:LEU:HD11	1:D:254:GLY:HA3	2.02	0.41
1:D:223:ARG:NH2	1:D:224:LYS:NZ	2.68	0.41
1:B:215:GLU:N	5:B:1274:ACT:H3	2.35	0.41
1:A:236:GLN:HE21	1:B:250[A]:GLN:CD	2.24	0.41
1:A:2:GLU:HG2	1:A:3:ALA:H	1.84	0.41
1:C:15:ILE:HB	2:C:1271:NAP:H51N	2.02	0.41
1:C:250[A]:GLN:CG	1:D:236:GLN:HE21	2.33	0.41
1:B:69:LEU:HD22	1:B:73:CYS:SG	2.60	0.41
1:C:153:ASN:OD1	1:C:250[B]:GLN:NE2	2.54	0.41
6:A:2166:HOH:O	1:B:250[A]:GLN:HG2	2.20	0.41
1:B:192:LEU:HB3	1:B:197:ILE:HB	2.03	0.41
1:B:160:CYS:HB3	6:B:2129:HOH:O	2.20	0.40
1:D:34:TYR:CZ	1:D:60:GLN:HB2	2.56	0.40
1:A:218:LYS:HZ2	5:A:1274:ACT:H1	1.86	0.40
1:C:242:ILE:HA	1:C:245:VAL:HG22	2.04	0.40
3:B:1272:MTX:HM1	3:B:1272:MTX:H15	1.82	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	252/268 (94%)	243 (96%)	9 (4%)	0	100	100
1	B	253/268 (94%)	244 (96%)	9 (4%)	0	100	100
1	C	261/268 (97%)	251 (96%)	10 (4%)	0	100	100
1	D	255/268 (95%)	244 (96%)	11 (4%)	0	100	100
All	All	1021/1072 (95%)	982 (96%)	39 (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	205/212 (97%)	194 (95%)	11 (5%)	27	31
1	B	207/212 (98%)	191 (92%)	16 (8%)	16	16
1	C	211/212 (100%)	195 (92%)	16 (8%)	16	16
1	D	207/212 (98%)	190 (92%)	17 (8%)	14	13
All	All	830/848 (98%)	770 (93%)	60 (7%)	22	18

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	44	LEU
1	A	50	LYS
1	A	58	VAL
1	A	60	GLN
1	A	69	LEU
1	A	159	LEU
1	A	229	ARG
1	A	242	ILE
1	A	250[A]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	250[B]	GLN
1	B	2	GLU
1	B	44	LEU
1	B	58	VAL
1	B	67[A]	ASN
1	B	67[B]	ASN
1	B	69	LEU
1	B	104	GLN
1	B	159	LEU
1	B	190	LEU
1	B	217[A]	GLU
1	B	217[B]	GLU
1	B	229	ARG
1	B	230	ARG
1	B	242	ILE
1	B	257[A]	ILE
1	B	257[B]	ILE
1	C	42	VAL
1	C	44	LEU
1	C	50	LYS
1	C	58	VAL
1	C	69	LEU
1	C	86	ARG
1	C	104[A]	GLN
1	C	104[B]	GLN
1	C	124[A]	ILE
1	C	124[B]	ILE
1	C	159	LEU
1	C	166	GLN
1	C	190	LEU
1	C	216	GLU
1	C	231	GLU
1	C	242	ILE
1	D	13	LYS
1	D	39	GLU
1	D	44	LEU
1	D	46	ASP
1	D	58	VAL
1	D	69	LEU
1	D	124[A]	ILE
1	D	124[B]	ILE
1	D	140	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	LYS
1	D	159	LEU
1	D	229	ARG
1	D	242	ILE
1	D	255[A]	SER
1	D	255[B]	SER
1	D	257[A]	ILE
1	D	257[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	B	104	GLN
1	B	236	GLN
1	C	35	HIS
1	D	67	ASN
1	D	104	GLN
1	D	112	ASN
1	D	236	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CAF	A	168	1	3,9,10	0.90	0	1,12,14	2.30	1 (100%)
1	CAF	A	59	1	3,9,10	0.70	0	1,12,14	2.17	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CAF	B	168	1	3,9,10	0.97	0	1,12,14	2.15	1 (100%)
1	CAF	B	59	1	3,9,10	0.84	0	1,12,14	2.61	1 (100%)
1	CAF	C	168	1	3,9,10	0.79	0	1,12,14	2.47	1 (100%)
1	CAF	C	59	1	3,9,10	0.93	0	1,12,14	2.20	1 (100%)
1	CAF	D	168	1	3,9,10	0.92	0	1,12,14	2.60	1 (100%)
1	CAF	D	59	1	3,9,10	0.78	0	1,12,14	1.91	0

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	CAF	A	168	1	-	0/0/8/10	0/0/0/0
1	CAF	A	59	1	-	0/0/8/10	0/0/0/0
1	CAF	B	168	1	-	0/0/8/10	0/0/0/0
1	CAF	B	59	1	-	0/0/8/10	0/0/0/0
1	CAF	C	168	1	-	0/0/8/10	0/0/0/0
1	CAF	C	59	1	-	0/0/8/10	0/0/0/0
1	CAF	D	168	1	-	0/0/8/10	0/0/0/0
1	CAF	D	59	1	-	0/0/8/10	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	CAF	O-C-CA	-2.61	118.70	125.49
1	D	168	CAF	O-C-CA	-2.60	118.70	125.49
1	C	168	CAF	O-C-CA	-2.47	119.04	125.49
1	A	168	CAF	O-C-CA	-2.30	119.51	125.49
1	C	59	CAF	O-C-CA	-2.20	119.77	125.49
1	A	59	CAF	O-C-CA	-2.17	119.84	125.49
1	B	168	CAF	O-C-CA	-2.15	119.90	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	59	CAF	3	0
1	B	168	CAF	2	0
1	B	59	CAF	3	0
1	C	168	CAF	1	0
1	C	59	CAF	1	0
1	D	59	CAF	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	A	1271	-	42,52,52	1.53	3 (7%)	54,80,80	1.96	8 (14%)
3	MTX	A	1272	-	27,35,35	2.02	4 (14%)	30,49,49	1.62	4 (13%)
5	ACT	A	1274	-	1,3,3	0.62	0	0,3,3	0.00	-
2	NAP	B	1271	-	42,52,52	1.50	3 (7%)	54,80,80	2.08	6 (11%)
3	MTX	B	1272	-	27,35,35	2.13	5 (18%)	30,49,49	1.47	5 (16%)
5	ACT	B	1274	-	1,3,3	0.41	0	0,3,3	0.00	-
2	NAP	C	1271	-	42,52,52	1.59	3 (7%)	54,80,80	2.02	9 (16%)
3	MTX	C	1272	-	27,35,35	2.13	5 (18%)	30,49,49	1.57	3 (10%)
2	NAP	D	1271	-	42,52,52	1.70	3 (7%)	54,80,80	1.93	7 (12%)
3	MTX	D	1272	-	27,35,35	2.21	4 (14%)	30,49,49	1.63	4 (13%)

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	1271	-	-	0/27/67/67	0/5/5/5
3	MTX	A	1272	-	-	0/19/25/25	0/3/3/3
5	ACT	A	1274	-	-	0/0/0/0	0/0/0/0
2	NAP	B	1271	-	-	0/27/67/67	0/5/5/5
3	MTX	B	1272	-	-	0/19/25/25	0/3/3/3
5	ACT	B	1274	-	-	0/0/0/0	0/0/0/0
2	NAP	C	1271	-	-	0/27/67/67	0/5/5/5
3	MTX	C	1272	-	-	0/19/25/25	0/3/3/3
2	NAP	D	1271	-	-	0/27/67/67	0/5/5/5
3	MTX	D	1272	-	-	0/19/25/25	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1272	MTX	C4-N3	2.02	1.38	1.33
3	C	1272	MTX	C2-N3	2.02	1.39	1.35
3	A	1272	MTX	C4-N3	2.03	1.38	1.33
2	C	1271	NAP	C2A-N1A	2.12	1.37	1.33
3	B	1272	MTX	C4-N3	2.14	1.38	1.33
3	B	1272	MTX	C2-N3	2.18	1.39	1.35
2	A	1271	NAP	C2A-N1A	2.29	1.38	1.33
3	C	1272	MTX	C4-N3	2.35	1.39	1.33
2	D	1271	NAP	C2A-N1A	2.54	1.38	1.33
2	B	1271	NAP	C2A-N1A	2.78	1.39	1.33
3	A	1272	MTX	C6-N5	2.85	1.38	1.32
3	B	1272	MTX	C6-N5	3.30	1.39	1.32
3	C	1272	MTX	C6-N5	3.38	1.39	1.32
3	C	1272	MTX	C7-N8	3.38	1.37	1.31
3	D	1272	MTX	C6-N5	3.49	1.39	1.32
2	C	1271	NAP	C2A-N3A	3.53	1.38	1.32
2	D	1271	NAP	C2A-N3A	3.60	1.38	1.32
2	A	1271	NAP	C2A-N3A	3.64	1.38	1.32
3	A	1272	MTX	C7-N8	3.67	1.38	1.31
3	D	1272	MTX	C7-N8	3.80	1.38	1.31
3	B	1272	MTX	C7-N8	3.85	1.38	1.31
2	B	1271	NAP	C2A-N3A	3.85	1.39	1.32
2	B	1271	NAP	O7N-C7N	7.31	1.39	1.24
2	A	1271	NAP	O7N-C7N	7.79	1.40	1.24
2	C	1271	NAP	O7N-C7N	7.89	1.41	1.24
3	A	1272	MTX	O-C	8.54	1.40	1.23
3	B	1272	MTX	O-C	8.70	1.40	1.23
2	D	1271	NAP	O7N-C7N	8.80	1.42	1.24
3	C	1272	MTX	O-C	8.89	1.41	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1272	MTX	O-C	9.17	1.41	1.23

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1271	NAP	N3A-C2A-N1A	-11.23	120.29	128.89
2	D	1271	NAP	N3A-C2A-N1A	-11.22	120.31	128.89
2	B	1271	NAP	N3A-C2A-N1A	-11.05	120.43	128.89
2	C	1271	NAP	N3A-C2A-N1A	-10.85	120.58	128.89
3	A	1272	MTX	N1-C2-N3	-4.86	120.05	127.44
3	D	1272	MTX	N1-C2-N3	-4.76	120.19	127.44
3	B	1272	MTX	N1-C2-N3	-4.76	120.19	127.44
3	C	1272	MTX	N1-C2-N3	-4.75	120.21	127.44
2	B	1271	NAP	C4B-O4B-C1B	-4.35	104.94	109.72
2	D	1271	NAP	C4B-O4B-C1B	-3.55	105.82	109.72
2	D	1271	NAP	PN-O3-PA	-2.70	125.14	132.73
2	C	1271	NAP	C1B-N9A-C4A	-2.65	122.95	126.94
2	C	1271	NAP	C4A-C5A-N7A	-2.49	107.19	109.48
2	B	1271	NAP	C1B-N9A-C4A	-2.48	123.21	126.94
2	A	1271	NAP	C4A-C5A-N7A	-2.40	107.27	109.48
2	C	1271	NAP	C4B-O4B-C1B	-2.26	107.24	109.72
2	C	1271	NAP	PN-O3-PA	-2.25	126.42	132.73
2	A	1271	NAP	PN-O3-PA	-2.22	126.49	132.73
2	C	1271	NAP	O7N-C7N-N7N	-2.20	119.50	122.59
2	A	1271	NAP	O7N-C7N-C3N	-2.15	117.24	119.59
2	D	1271	NAP	C4A-C5A-N7A	-2.03	107.61	109.48
2	D	1271	NAP	C1B-N9A-C4A	-2.02	123.90	126.94
2	A	1271	NAP	C4B-O4B-C1B	-2.00	107.52	109.72
3	B	1272	MTX	NA2-C2-N3	2.08	120.65	117.20
3	B	1272	MTX	C7-N8-C8A	2.20	119.52	116.93
3	B	1272	MTX	N8-C8A-N1	2.40	119.58	116.14
3	D	1272	MTX	N8-C8A-N1	2.49	119.70	116.14
3	A	1272	MTX	C9-C6-N5	2.66	121.46	117.11
3	B	1272	MTX	C9-C6-N5	2.71	121.54	117.11
2	A	1271	NAP	C3N-C7N-N7N	2.77	120.85	117.82
3	A	1272	MTX	N8-C8A-N1	2.82	120.17	116.14
3	C	1272	MTX	C7-N8-C8A	2.96	120.42	116.93
3	A	1272	MTX	C7-N8-C8A	3.28	120.79	116.93
2	D	1271	NAP	O4D-C1D-N1N	3.29	111.74	108.13
3	D	1272	MTX	C7-N8-C8A	3.36	120.89	116.93
3	D	1272	MTX	C9-C6-N5	3.37	122.62	117.11
2	A	1271	NAP	O4D-C1D-N1N	3.49	111.97	108.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1271	NAP	O4B-C1B-N9A	3.58	115.58	108.10
2	D	1271	NAP	O4B-C1B-N9A	3.67	115.77	108.10
2	C	1271	NAP	O4B-C1B-N9A	3.70	115.85	108.10
2	B	1271	NAP	C3N-C7N-N7N	3.90	122.09	117.82
2	C	1271	NAP	C3N-C7N-N7N	4.00	122.20	117.82
2	A	1271	NAP	O4B-C1B-N9A	4.25	116.98	108.10
3	C	1272	MTX	C9-C6-N5	4.26	124.08	117.11
2	B	1271	NAP	O4D-C1D-N1N	4.44	113.01	108.13
2	C	1271	NAP	O4D-C1D-N1N	4.45	113.02	108.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1274	ACT	5	0
3	B	1272	MTX	3	0
5	B	1274	ACT	5	0
2	C	1271	NAP	1	0
3	C	1272	MTX	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 ⓘ

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	251/268 (93%)	-0.32	8 (3%) 51 50	16, 21, 33, 48	0
1	B	252/268 (94%)	-0.38	7 (2%) 56 55	15, 21, 33, 48	0
1	C	258/268 (96%)	-0.24	12 (4%) 35 34	16, 22, 37, 50	0
1	D	255/268 (95%)	-0.21	13 (5%) 32 31	14, 22, 37, 62	0
All	All	1016/1072 (94%)	-0.29	40 (3%) 43 42	14, 22, 36, 62	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	ASN	8.0
1	C	144	GLY	6.9
1	D	106	ASP	6.5
1	C	105	GLY	6.1
1	D	107	HIS	5.8
1	D	112	ASN	5.2
1	D	105	GLY	5.0
1	B	104	GLN	4.7
1	B	113	GLY	4.6
1	D	113	GLY	4.5
1	A	113	GLY	4.0
1	D	144	GLY	3.9
1	B	150	THR	3.8
1	D	104	GLN	3.8
1	C	145	THR	3.5
1	C	143	LYS	3.2
1	C	113	GLY	3.1
1	B	143	LYS	3.0
1	B	151	SER	2.9
1	B	2	GLU	2.8
1	A	104	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	144	GLY	2.7
1	D	2	GLU	2.5
1	A	152	SER	2.5
1	C	2	GLU	2.5
1	D	151	SER	2.4
1	A	151	SER	2.4
1	D	216	GLU	2.3
1	D	223	ARG	2.3
1	C	104[A]	GLN	2.2
1	A	51	GLU	2.2
1	C	151	SER	2.2
1	C	150	THR	2.2
1	C	148	ASN	2.2
1	A	50	LYS	2.1
1	A	143	LYS	2.1
1	C	91	VAL	2.1
1	D	91	VAL	2.1
1	C	149	CYS	2.1
1	D	143	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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 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(Å ²)	Q<0.9
1	CAF	A	59	10/11	0.97	0.10	-	28,30,44,46	0
1	CAF	B	168	10/11	0.96	0.12	-	23,24,32,32	4
1	CAF	C	59	10/11	0.97	0.11	-	24,26,34,34	0
1	CAF	D	168	10/11	0.90	0.14	-	27,29,38,39	4
1	CAF	A	168	10/11	0.95	0.11	-	25,27,37,38	4
1	CAF	B	59	10/11	0.97	0.10	-	23,25,37,38	0
1	CAF	C	168	10/11	0.91	0.16	-	24,27,37,38	4
1	CAF	D	59	10/11	0.97	0.10	-	24,26,35,37	0

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 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(\AA^2)	Q<0.9
5	ACT	A	1274	4/4	0.91	0.17	1.77	37,38,38,38	0
3	MTX	C	1272	33/33	0.92	0.14	0.99	16,25,36,37	0
5	ACT	B	1274	4/4	0.95	0.13	0.98	23,23,23,24	0
3	MTX	B	1272	33/33	0.95	0.10	0.84	14,22,30,32	0
3	MTX	D	1272	33/33	0.93	0.13	0.56	16,26,35,37	0
3	MTX	A	1272	33/33	0.94	0.11	0.16	19,24,30,32	0
2	NAP	B	1271	48/48	0.98	0.09	-0.65	14,17,20,21	0
2	NAP	C	1271	48/48	0.97	0.09	-0.75	14,17,20,21	0
2	NAP	A	1271	48/48	0.98	0.08	-0.99	14,19,21,22	0
2	NAP	D	1271	48/48	0.98	0.08	-1.05	15,18,22,24	0
4	NI	B	1273	1/1	0.99	0.13	-	43,43,43,43	1
4	NI	A	1273	1/1	0.95	0.21	-	49,49,49,49	1

6.5 Other polymers [i](#)

There are no such residues in this entry.