



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:44 PM GMT

PDB ID : 1LRT
Title : CRYSTAL STRUCTURE OF TERNARY COMPLEX OF TRITRICHOMONAS FOETUS INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE: STRUCTURAL CHARACTERIZATION OF NAD⁺ SITE IN MICROBIAL ENZYME
Authors : Gan, L.; Petsko, G.A.; Hedstrom, L.
Deposited on : 2002-05-15
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

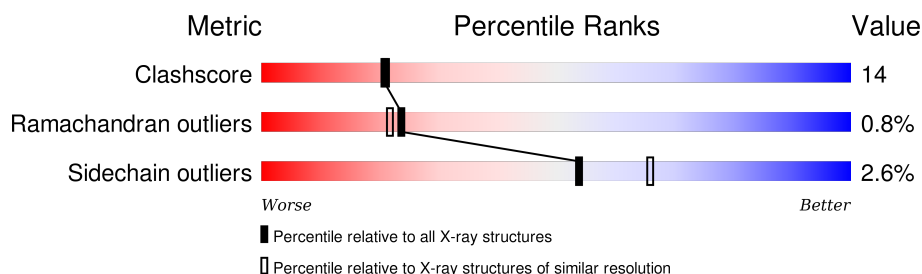
1 Overall quality at a glance

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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	376	 69% 19% • 10%
1	B	376	 63% 24% • 11%
1	C	376	 67% 20% • 11%
1	D	376	 64% 23% • 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11238 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.

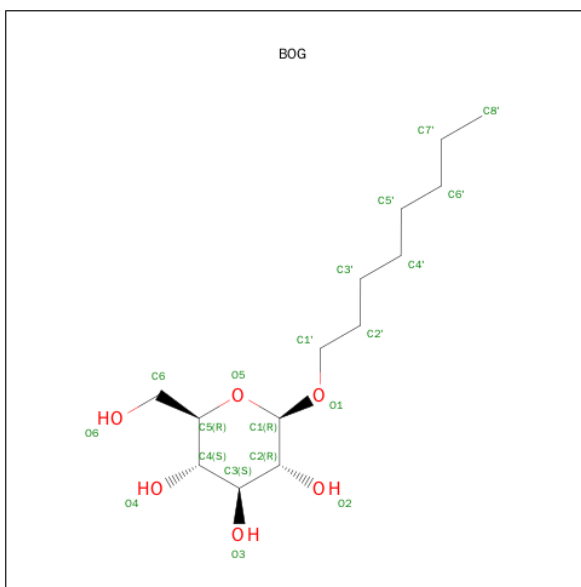
- Molecule 1 is a protein called INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2583	1638	437	493	15			
1	B	334	Total	C	N	O	S	0	0	0
			2554	1621	433	485	15			
1	C	334	Total	C	N	O	S	0	0	0
			2554	1621	433	485	15			
1	D	340	Total	C	N	O	S	0	0	0
			2600	1649	442	494	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ASP	GLU	SEE REMARK 999	UNP P50097
B	279	ASP	GLU	SEE REMARK 999	UNP P50097
C	279	ASP	GLU	SEE REMARK 999	UNP P50097
D	279	ASP	GLU	SEE REMARK 999	UNP P50097

- Molecule 2 is INOSINE-5'-MONOPHOSPHATE (three-letter code: BOG) (formula: C₁₄H₂₈O₆).

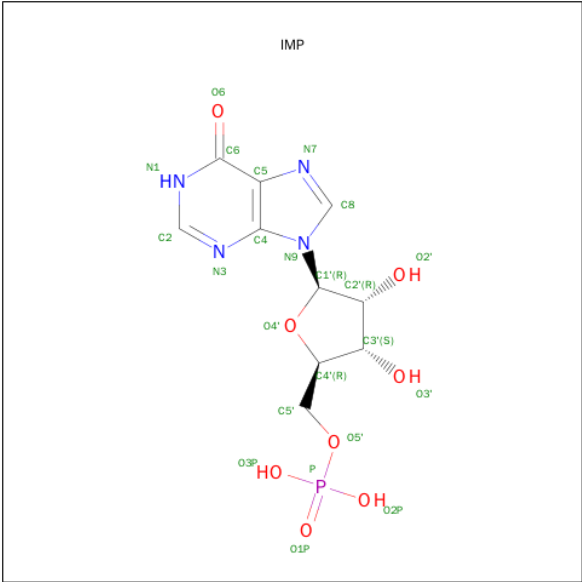


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

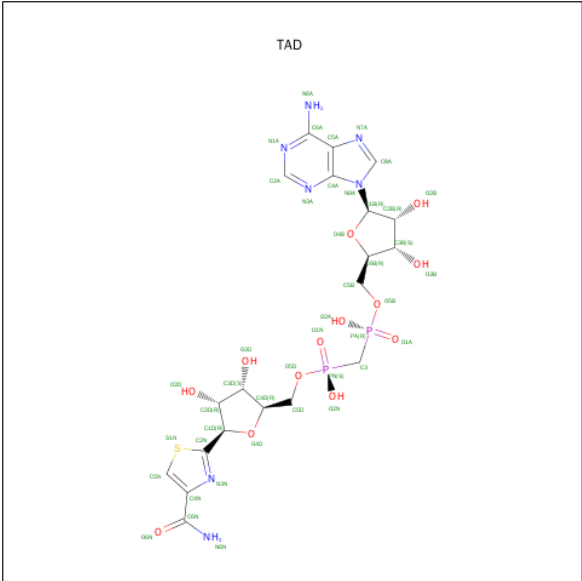
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		

- Molecule 4 is INOSINIC ACID (three-letter code: IMP) (formula: C₁₀H₁₃N₄O₈P).



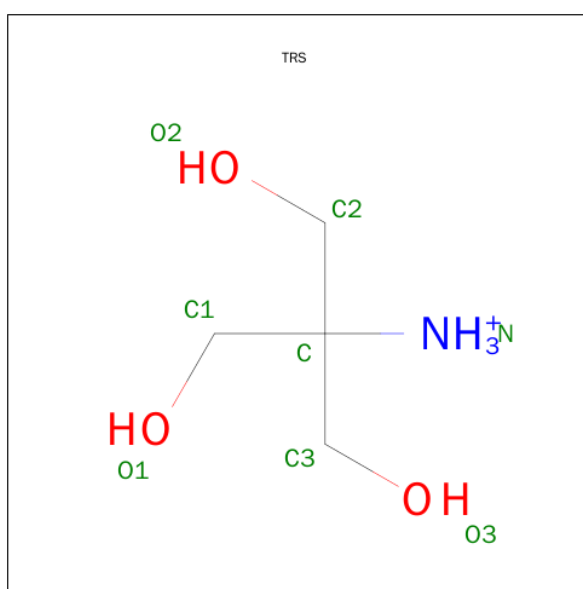
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
4	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 5 is BETA-METHYLENE-THIAZOLE-4-CARBOXYAMIDE-ADENINE DINUCLEOTIDE (three-letter code: TAD) (formula: C₂₀H₂₇N₇O₁₃P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	
5	B	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	
5	C	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	
5	D	1	Total	C	N	O	P	S	
			43	20	7	13	2	1	

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O		
			8	4	1	3	0	0
6	A	1	Total	C	N	O		
			8	4	1	3	0	0
6	C	1	Total	C	N	O		
			8	4	1	3	0	0
6	B	1	Total	C	N	O		
			8	4	1	3	0	0
6	D	1	Total	C	N	O		
			8	4	1	3	0	0
6	C	1	Total	C	N	O		
			8	4	1	3	0	0
6	D	1	Total	C	N	O		
			8	4	1	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 8	C 4	N 1	O 3	0	0
6	B	1	Total 8	C 4	N 1	O 3	0	0
6	D	1	Total 8	C 4	N 1	O 3	0	0
6	A	1	Total 8	C 4	N 1	O 3	0	0
6	B	1	Total 8	C 4	N 1	O 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	160	Total 160	O 160	0	0
7	B	128	Total 128	O 128	0	0
7	C	122	Total 122	O 122	0	0
7	D	133	Total 133	O 133	0	0

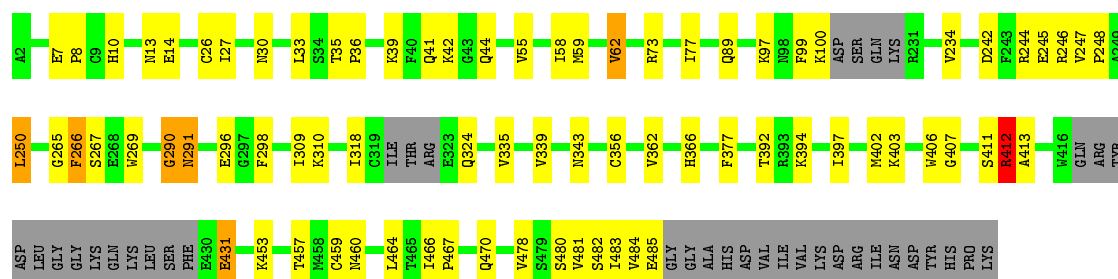
3 Residue-property plots

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.

Note EDS was not executed.

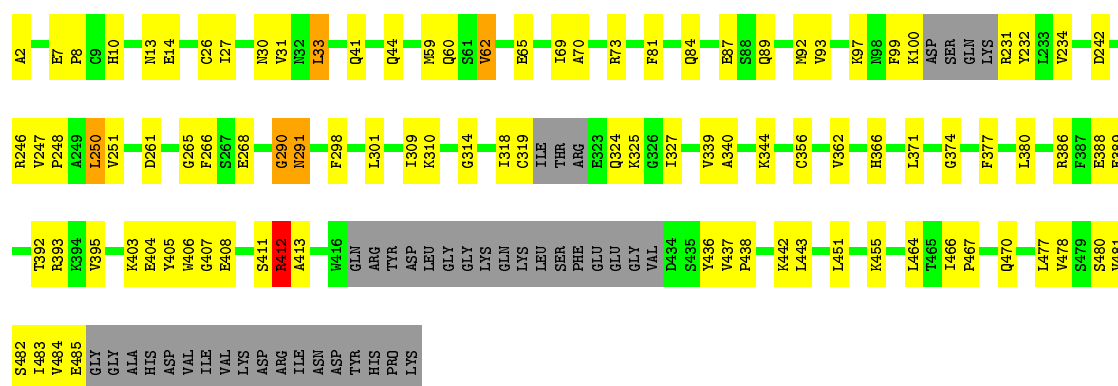
• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain A: 



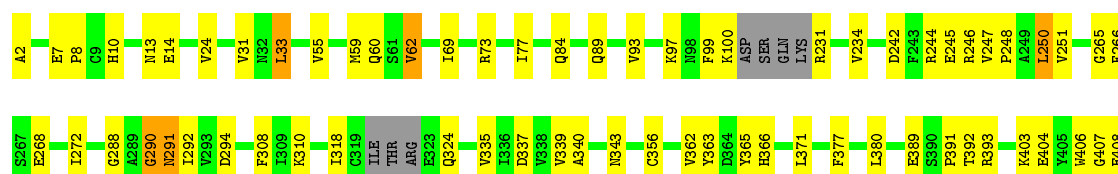
• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain B: 



• Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE

Chain C: 





PRO
LYS

● Molecule 1: INOSINE-5'-MONOPHOSPHATE DEHYDROGENASE



ILE
VAL
LYS
ASP
ARG
ILE
ASN
ASP
TYR
HIS
PRO
LYS

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.14Å 112.37Å 162.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 2.20	Depositor
% Data completeness (in resolution range)	91.4 (29.86-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11238	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

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: TAD, IMP, K, TRS, BOG

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	0.34	0/2627	0.61	1/3541 (0.0%)
1	B	0.32	0/2598	0.59	1/3502 (0.0%)
1	C	0.33	0/2598	0.60	1/3502 (0.0%)
1	D	0.33	0/2645	0.60	1/3567 (0.0%)
All	All	0.33	0/10468	0.60	4/14112 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLY	N-CA-C	6.85	130.22	113.10
1	C	290	GLY	N-CA-C	6.83	130.18	113.10
1	D	290	GLY	N-CA-C	6.76	129.99	113.10
1	B	290	GLY	N-CA-C	6.16	128.50	113.10

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	2583	0	2572	65	0
1	B	2554	0	2548	82	0
1	C	2554	0	2548	71	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2600	0	2598	100	0
2	A	40	0	56	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	23	0	11	0	0
4	B	23	0	11	0	0
4	C	23	0	11	0	0
4	D	23	0	11	2	0
5	A	43	0	24	0	0
5	B	43	0	24	1	0
5	C	43	0	24	0	0
5	D	43	0	24	3	0
6	A	32	0	48	5	0
6	B	24	0	36	2	0
6	C	16	0	24	4	0
6	D	24	0	36	7	0
7	A	160	0	0	3	0
7	B	128	0	0	0	0
7	C	122	0	0	2	0
7	D	133	0	0	1	0
All	All	11238	0	10606	307	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 14.

All (307) 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:D:322:ARG:HH22	5:D:904:TAD:H5N	1.25	1.02
1:D:322:ARG:HB3	1:D:326:GLY:H	1.35	0.89
1:D:322:ARG:HG2	1:D:327:ILE:H	1.36	0.89
1:C:7:GLU:HG3	1:C:8:PRO:HD2	1.60	0.83
1:C:343:ASN:ND2	6:C:605:TRS:H11	1.93	0.83
1:D:320:ILE:HD13	1:D:320:ILE:H	1.44	0.82
1:B:41:GLN:HB3	1:B:44:GLN:HE21	1.44	0.82
1:D:433:VAL:HG12	1:D:434:ASP:H	1.42	0.82
1:C:362:VAL:H	1:C:366:HIS:HD2	1.27	0.82
1:D:322:ARG:HB3	1:D:326:GLY:N	1.95	0.80
1:B:89:GLN:HG2	1:B:250:LEU:HD11	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:ARG:NH2	5:D:904:TAD:H5N	1.97	0.79
1:B:59:MET:HB2	1:B:62:VAL:HG13	1.66	0.78
1:A:411:SER:O	1:A:412:ARG:HB3	1.82	0.77
1:C:343:ASN:HD22	6:C:605:TRS:H11	1.50	0.77
1:A:59:MET:HB2	1:A:62:VAL:HG13	1.68	0.76
6:A:607:TRS:HO1	1:D:2:ALA:N	1.85	0.75
1:D:290:GLY:O	1:D:291:ASN:HB2	1.88	0.72
1:A:412:ARG:HG3	1:A:413:ALA:N	2.02	0.71
1:B:242:ASP:OD1	1:B:246:ARG:HD2	1.91	0.71
1:A:291:ASN:HA	1:A:310:LYS:O	1.91	0.71
1:B:291:ASN:HA	1:B:310:LYS:O	1.92	0.70
1:A:265:GLY:HA3	1:A:290:GLY:HA2	1.73	0.70
1:C:412:ARG:HG3	1:C:413:ALA:N	2.06	0.69
1:B:10:HIS:HD2	1:B:14:GLU:OE1	1.76	0.69
1:C:59:MET:HB2	1:C:62:VAL:HG13	1.74	0.68
1:D:291:ASN:HA	1:D:310:LYS:O	1.94	0.68
1:C:10:HIS:HD2	1:C:14:GLU:OE1	1.77	0.68
1:B:362:VAL:H	1:B:366:HIS:HD2	1.41	0.68
1:D:409:GLY:HA3	1:D:431:GLU:HB2	1.77	0.67
1:B:7:GLU:HG3	1:B:8:PRO:HD2	1.76	0.67
1:C:290:GLY:O	1:C:291:ASN:HB2	1.93	0.67
1:C:291:ASN:HA	1:C:310:LYS:O	1.94	0.67
1:A:267:SER:HB3	6:A:600:TRS:H32	1.77	0.67
1:B:483:ILE:HD12	1:C:481:VAL:HG21	1.76	0.66
1:A:36:PRO:HB3	6:A:610:TRS:H21	1.76	0.66
1:D:318:ILE:HD12	1:D:407:GLY:CA	2.25	0.66
1:D:318:ILE:HD12	1:D:407:GLY:HA2	1.77	0.66
1:D:483:ILE:C	1:D:485:GLU:H	1.97	0.66
1:D:5:TYR:HB3	6:D:609:TRS:H11	1.76	0.66
1:B:265:GLY:HA3	1:B:290:GLY:HA2	1.77	0.66
1:C:324:GLN:O	1:D:453:LYS:HD3	1.96	0.66
1:A:290:GLY:O	1:A:291:ASN:HB2	1.96	0.65
1:C:483:ILE:HD12	1:D:481:VAL:HG21	1.76	0.65
1:A:481:VAL:HG21	1:D:483:ILE:HD12	1.79	0.65
1:D:362:VAL:H	1:D:366:HIS:HD2	1.44	0.65
1:B:290:GLY:O	1:B:291:ASN:HB2	1.96	0.64
1:C:483:ILE:C	1:C:485:GLU:H	2.01	0.64
1:D:265:GLY:HA3	1:D:290:GLY:HA2	1.80	0.64
1:D:411:SER:O	1:D:412:ARG:HB3	1.97	0.64
1:D:412:ARG:HG3	1:D:413:ALA:N	2.12	0.64
1:A:362:VAL:H	1:A:366:HIS:HD2	1.44	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HG2	1:B:231:ARG:HH11	1.63	0.64
1:B:388:GLU:HG2	1:B:442:LYS:NZ	2.13	0.64
1:C:99:PHE:O	1:C:100:LYS:HB2	1.98	0.63
1:D:406:TRP:CD1	1:D:412:ARG:HD2	2.32	0.63
1:A:397:ILE:HD12	1:A:402:MET:HG3	1.81	0.62
1:B:412:ARG:HG3	1:B:413:ALA:N	2.12	0.62
1:B:483:ILE:C	1:B:485:GLU:H	2.01	0.62
1:A:55:VAL:HG12	1:A:77:ILE:HG22	1.82	0.62
1:A:457:THR:HG23	1:D:327:ILE:HD11	1.80	0.61
1:B:324:GLN:O	1:C:453:LYS:HD3	2.00	0.61
1:A:99:PHE:O	1:A:100:LYS:HB2	2.00	0.61
1:A:10:HIS:HD2	1:A:14:GLU:OE1	1.83	0.61
1:D:322:ARG:HG2	1:D:327:ILE:N	2.11	0.61
1:D:433:VAL:HG12	1:D:434:ASP:N	2.13	0.60
1:B:393:ARG:HG2	1:B:404:GLU:OE1	2.01	0.60
1:D:7:GLU:HG3	1:D:8:PRO:HD2	1.83	0.60
1:D:322:ARG:HH22	5:D:904:TAD:C5N	2.06	0.60
1:C:231:ARG:HH11	1:C:231:ARG:HG2	1.66	0.60
1:A:242:ASP:OD1	1:A:246:ARG:HD2	2.01	0.60
1:C:89:GLN:HG2	1:C:250:LEU:HD11	1.84	0.60
1:C:265:GLY:HA3	1:C:290:GLY:HA2	1.83	0.60
1:A:483:ILE:C	1:A:485:GLU:H	2.04	0.60
1:D:322:ARG:CG	1:D:327:ILE:H	2.09	0.59
1:D:59:MET:HE3	1:D:318:ILE:HD11	1.83	0.59
1:D:73:ARG:HH21	1:D:99:PHE:HE2	1.49	0.59
1:A:266:PHE:CE2	1:A:296:GLU:HG2	2.37	0.59
1:B:2:ALA:N	6:C:605:TRS:HO3	2.00	0.59
1:A:478:VAL:HG12	1:A:482:SER:HB2	1.85	0.59
1:C:13:ASN:ND2	1:C:366:HIS:CE1	2.71	0.58
1:C:480:SER:O	1:C:484:VAL:HG23	2.03	0.58
1:D:478:VAL:HG12	1:D:482:SER:HB2	1.84	0.58
1:A:394:LYS:HG2	1:A:403:LYS:HG2	1.86	0.57
1:B:97:LYS:HD3	1:B:234:VAL:HG12	1.85	0.57
1:B:65:GLU:HG3	1:B:92:MET:HG2	1.86	0.57
1:B:247:VAL:O	1:B:251:VAL:HG23	2.04	0.57
1:B:59:MET:HB2	1:B:62:VAL:CG1	2.32	0.57
1:A:483:ILE:HD12	1:B:481:VAL:HG21	1.86	0.57
1:D:322:ARG:HB3	1:D:326:GLY:CA	2.36	0.56
1:D:7:GLU:CG	1:D:8:PRO:HD2	2.34	0.56
1:D:265:GLY:HA3	1:D:290:GLY:CA	2.36	0.56
1:C:483:ILE:C	1:C:485:GLU:N	2.59	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:PHE:O	1:C:100:LYS:CB	2.53	0.56
1:D:320:ILE:HD13	1:D:320:ILE:N	2.18	0.55
1:A:480:SER:O	1:A:484:VAL:HG23	2.06	0.55
1:D:466:ILE:O	1:D:470:GLN:HG3	2.05	0.55
1:D:322:ARG:N	1:D:322:ARG:HD2	2.22	0.55
1:C:380:LEU:N	1:C:380:LEU:HD12	2.20	0.55
1:B:340:ALA:O	1:B:344:LYS:HG3	2.06	0.55
1:B:318:ILE:HD12	1:B:407:GLY:CA	2.35	0.55
1:D:406:TRP:NE1	1:D:412:ARG:HD2	2.22	0.55
1:B:99:PHE:O	1:B:100:LYS:HB2	2.07	0.55
1:C:318:ILE:HD12	1:C:407:GLY:CA	2.36	0.55
1:D:483:ILE:C	1:D:485:GLU:N	2.60	0.55
1:B:393:ARG:HG2	1:B:404:GLU:CD	2.27	0.55
1:C:2:ALA:N	6:D:606:TRS:HO1	2.05	0.55
1:A:406:TRP:NE1	1:A:412:ARG:HD2	2.23	0.54
1:D:99:PHE:O	1:D:100:LYS:HG3	2.08	0.54
1:D:340:ALA:O	1:D:344:LYS:HG3	2.07	0.54
1:A:59:MET:HB2	1:A:62:VAL:CG1	2.37	0.54
1:C:59:MET:HE3	1:C:318:ILE:HD11	1.90	0.54
1:D:26:CYS:SG	1:D:464:LEU:HD22	2.47	0.54
1:D:380:LEU:HD12	1:D:380:LEU:N	2.23	0.54
1:D:51:LYS:HB2	1:D:75:GLY:HA3	1.90	0.54
1:C:242:ASP:OD1	1:C:246:ARG:HD2	2.08	0.54
1:A:324:GLN:HE22	1:A:431:GLU:HA	1.72	0.54
1:B:99:PHE:O	1:B:100:LYS:CB	2.56	0.53
1:A:97:LYS:HD3	1:A:234:VAL:HG12	1.89	0.53
1:C:73:ARG:HH21	1:C:99:PHE:HE2	1.56	0.53
1:A:99:PHE:O	1:A:100:LYS:CB	2.56	0.53
1:D:356:CYS:HB2	1:D:377:PHE:CE2	2.44	0.53
1:B:484:VAL:HG12	1:B:484:VAL:O	2.08	0.53
1:C:392:THR:OG1	1:C:403:LYS:HE2	2.08	0.53
1:B:411:SER:O	1:B:412:ARG:HB3	2.08	0.53
1:A:324:GLN:HE22	1:A:431:GLU:C	2.11	0.53
1:A:318:ILE:HD12	1:A:407:GLY:CA	2.39	0.53
1:C:356:CYS:HB2	1:C:377:PHE:CE2	2.44	0.53
1:D:231:ARG:HH11	1:D:231:ARG:HG2	1.73	0.53
1:D:10:HIS:HD2	1:D:14:GLU:OE1	1.91	0.52
1:D:484:VAL:O	1:D:484:VAL:HG12	2.09	0.52
1:A:73:ARG:NH2	1:A:99:PHE:HE2	2.07	0.52
1:B:59:MET:HE3	1:B:318:ILE:HD11	1.91	0.52
1:D:97:LYS:HD3	1:D:234:VAL:HG12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:484:VAL:C	1:D:485:GLU:HG2	2.29	0.52
1:A:7:GLU:HG3	1:A:8:PRO:HD2	1.92	0.52
1:D:247:VAL:HB	1:D:248:PRO:HD3	1.92	0.52
1:B:395:VAL:HG21	1:B:436:TYR:CE2	2.44	0.52
1:B:483:ILE:C	1:B:485:GLU:N	2.63	0.52
1:C:484:VAL:HG12	1:C:484:VAL:O	2.09	0.52
1:A:484:VAL:HG12	1:A:484:VAL:O	2.11	0.51
1:B:231:ARG:HG2	1:B:231:ARG:NH1	2.26	0.51
1:A:483:ILE:C	1:A:485:GLU:N	2.63	0.51
1:A:356:CYS:HB2	1:A:377:PHE:CE2	2.46	0.51
1:B:13:ASN:ND2	1:B:366:HIS:CE1	2.79	0.51
1:A:26:CYS:SG	1:A:464:LEU:HD22	2.50	0.51
1:C:7:GLU:HG3	1:C:8:PRO:CD	2.37	0.50
1:D:320:ILE:O	1:D:322:ARG:N	2.44	0.50
1:B:380:LEU:HD12	1:B:380:LEU:N	2.26	0.50
1:C:60:GLN:HG3	1:C:408:GLU:OE2	2.11	0.50
1:D:99:PHE:O	1:D:100:LYS:CB	2.59	0.50
1:A:89:GLN:HG2	1:A:250:LEU:HD11	1.93	0.50
1:C:406:TRP:NE1	1:C:412:ARG:HD2	2.27	0.50
1:A:44:GLN:NE2	7:A:984:HOH:O	2.43	0.50
1:A:58:ILE:HD12	7:A:973:HOH:O	2.12	0.50
1:C:231:ARG:NH1	1:C:231:ARG:HG2	2.28	0.49
1:B:395:VAL:HG21	1:B:436:TYR:HE2	1.76	0.49
1:C:97:LYS:HD3	1:C:234:VAL:HG12	1.93	0.49
1:A:324:GLN:HE22	1:A:431:GLU:CA	2.26	0.49
1:A:453:LYS:HD3	1:D:324:GLN:O	2.11	0.49
1:B:389:GLU:N	1:B:389:GLU:OE1	2.45	0.49
1:C:484:VAL:C	1:C:485:GLU:HG2	2.32	0.49
1:A:324:GLN:NE2	1:A:431:GLU:HA	2.28	0.49
1:B:478:VAL:HG12	1:B:482:SER:HB2	1.94	0.49
1:A:73:ARG:HH21	1:A:99:PHE:HE2	1.58	0.49
1:D:62:VAL:CG2	1:D:63:SER:N	2.76	0.49
1:D:290:GLY:HA3	1:D:301:LEU:HD11	1.95	0.48
1:C:55:VAL:HG12	1:C:77:ILE:HG22	1.95	0.48
1:B:26:CYS:SG	1:B:464:LEU:HD22	2.53	0.48
1:C:413:ALA:O	1:C:416:TRP:HD1	1.95	0.48
1:D:484:VAL:O	1:D:485:GLU:HG2	2.14	0.48
1:A:247:VAL:HB	1:A:248:PRO:HD3	1.95	0.48
1:C:340:ALA:HA	6:C:605:TRS:O1	2.13	0.48
1:D:478:VAL:CG1	1:D:482:SER:HB2	2.43	0.48
1:B:480:SER:O	1:B:484:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLN:O	1:D:246:ARG:NH2	2.41	0.48
1:D:270:GLN:OE1	1:D:290:GLY:N	2.47	0.48
1:D:13:ASN:ND2	1:D:366:HIS:CE1	2.82	0.48
1:B:388:GLU:HG2	1:B:442:LYS:HZ1	1.78	0.48
1:B:392:THR:OG1	1:B:403:LYS:HE2	2.14	0.48
1:D:59:MET:CE	1:D:318:ILE:HD11	2.44	0.47
1:A:266:PHE:CZ	1:A:296:GLU:HG2	2.49	0.47
1:D:60:GLN:HG3	1:D:408:GLU:OE2	2.14	0.47
1:B:406:TRP:CD1	1:B:412:ARG:HD2	2.49	0.47
1:D:33:LEU:HD22	1:D:455:LYS:HE3	1.97	0.47
1:A:41:GLN:HG2	1:A:42:LYS:N	2.29	0.47
1:D:362:VAL:H	1:D:366:HIS:CD2	2.29	0.46
1:B:31:VAL:HG12	1:B:33:LEU:HD13	1.97	0.46
1:D:322:ARG:C	1:D:324:GLN:H	2.13	0.46
1:B:261:ASP:OD2	5:B:902:TAD:O3D	2.33	0.46
1:B:339:VAL:HG21	1:B:374:GLY:HA3	1.97	0.46
1:A:457:THR:HG23	1:D:327:ILE:CD1	2.45	0.46
1:A:35:THR:OG1	1:A:36:PRO:HD2	2.16	0.46
1:D:65:GLU:HG3	1:D:92:MET:HG2	1.96	0.46
1:C:69:ILE:O	1:C:73:ARG:HG3	2.16	0.46
1:D:99:PHE:O	1:D:100:LYS:HB2	2.16	0.46
1:D:458:MET:HG2	1:D:469:LEU:HD22	1.97	0.46
1:B:318:ILE:HD13	1:B:405:TYR:CE2	2.51	0.46
1:C:335:VAL:O	1:C:339:VAL:HG23	2.16	0.46
1:A:484:VAL:C	1:A:485:GLU:HG2	2.37	0.45
1:A:318:ILE:HD12	1:A:407:GLY:HA2	1.98	0.45
1:D:324:GLN:HE22	1:D:431:GLU:N	2.15	0.45
1:B:247:VAL:HB	1:B:248:PRO:HD3	1.99	0.45
1:B:60:GLN:HG3	1:B:408:GLU:OE2	2.17	0.45
1:A:13:ASN:ND2	1:A:366:HIS:CE1	2.85	0.45
1:A:466:ILE:O	1:A:470:GLN:HG3	2.16	0.45
1:C:10:HIS:CD2	1:C:14:GLU:OE1	2.65	0.45
1:D:39:LYS:HA	1:D:354:PRO:HD3	1.98	0.45
1:B:14:GLU:HA	1:B:483:ILE:HD11	1.99	0.45
1:D:466:ILE:HB	1:D:467:PRO:HD3	1.99	0.45
1:C:31:VAL:HG12	1:C:33:LEU:HD13	1.98	0.45
1:B:298:PHE:CE1	1:B:309:ILE:HD12	2.51	0.45
1:D:319:CYS:SG	1:D:322:ARG:NH1	2.90	0.45
1:B:70:ALA:HB2	1:B:389:GLU:HG2	1.98	0.45
1:B:466:ILE:HB	1:B:467:PRO:HD3	1.99	0.45
1:D:33:LEU:HD22	1:D:455:LYS:CE	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:THR:HG22	1:D:321:THR:O	2.17	0.45
1:C:443:LEU:C	1:C:443:LEU:HD23	2.37	0.45
1:B:268:GLU:OE2	1:C:24:VAL:HG13	2.18	0.44
1:B:314:GLY:HA2	1:B:319:CYS:SG	2.57	0.44
1:B:327:ILE:HD11	1:C:457:THR:HG23	1.98	0.44
1:B:93:VAL:O	1:B:97:LYS:HG2	2.16	0.44
1:B:60:GLN:HA	1:B:81:PHE:CD2	2.53	0.44
1:D:432:GLY:HA3	4:D:804:IMP:O6	2.16	0.44
1:B:290:GLY:HA3	1:B:301:LEU:CD1	2.48	0.44
1:D:5:TYR:HB3	6:D:609:TRS:H21	2.00	0.44
1:B:339:VAL:HG12	6:B:608:TRS:O2	2.17	0.44
1:D:395:VAL:HG21	1:D:436:TYR:CE2	2.52	0.44
1:C:292:ILE:C	1:C:292:ILE:HD12	2.37	0.44
1:C:389:GLU:N	1:C:389:GLU:OE1	2.50	0.44
1:C:247:VAL:HB	1:C:248:PRO:HD3	1.98	0.44
1:A:26:CYS:C	1:A:459:CYS:SG	2.95	0.44
1:C:268:GLU:O	1:C:272:ILE:HG13	2.18	0.44
1:A:343:ASN:ND2	6:A:607:TRS:H21	2.31	0.44
1:C:484:VAL:O	1:C:485:GLU:HG2	2.18	0.44
1:C:371:LEU:O	1:C:470:GLN:HG2	2.18	0.44
1:D:397:ILE:HD12	1:D:402:MET:HG3	2.00	0.44
1:B:69:ILE:O	1:B:73:ARG:HG3	2.18	0.44
1:A:245:GLU:OE2	2:A:752:BOG:O4	2.31	0.43
1:B:386:ARG:HB3	1:B:438:PRO:O	2.17	0.43
1:C:244:ARG:HB2	7:C:916:HOH:O	2.17	0.43
1:C:59:MET:CE	1:C:318:ILE:HD11	2.48	0.43
1:B:84:GLN:O	1:B:246:ARG:NH2	2.41	0.43
1:D:292:ILE:C	1:D:292:ILE:HD12	2.39	0.43
1:C:33:LEU:HD22	1:C:455:LYS:HE3	2.00	0.43
1:D:443:LEU:HD23	1:D:443:LEU:C	2.39	0.43
1:D:69:ILE:HG23	1:D:232:TYR:CE1	2.54	0.43
1:C:318:ILE:HD12	1:C:407:GLY:HA2	2.00	0.43
1:B:443:LEU:HD23	1:B:443:LEU:C	2.38	0.43
1:D:34:SER:HA	1:D:50:LEU:O	2.19	0.43
1:C:288:GLY:HA3	1:C:308:PHE:CZ	2.53	0.43
1:B:27:ILE:HG12	1:B:30:ASN:ND2	2.34	0.43
1:D:371:LEU:O	1:D:470:GLN:HG2	2.19	0.42
1:C:247:VAL:O	1:C:251:VAL:HG23	2.19	0.42
1:C:363:TYR:O	1:C:366:HIS:HB2	2.19	0.42
1:C:483:ILE:O	1:C:485:GLU:N	2.52	0.42
1:D:319:CYS:HB2	4:D:804:IMP:H2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:SER:O	1:D:484:VAL:HG23	2.19	0.42
1:C:33:LEU:HD22	1:C:455:LYS:CE	2.49	0.42
1:A:7:GLU:CG	1:A:8:PRO:HD2	2.50	0.42
1:A:39:LYS:NZ	6:A:601:TRS:H12	2.34	0.42
1:B:356:CYS:HB2	1:B:377:PHE:CE2	2.55	0.42
1:D:322:ARG:CB	1:D:326:GLY:H	2.20	0.42
1:D:5:TYR:HB3	6:D:609:TRS:C1	2.45	0.42
1:C:84:GLN:O	1:C:246:ARG:NH2	2.39	0.42
1:A:244:ARG:HB2	7:A:953:HOH:O	2.19	0.42
1:B:318:ILE:HD12	1:B:407:GLY:HA2	2.00	0.42
1:B:386:ARG:HG2	1:B:437:VAL:HB	2.01	0.42
1:A:460:ASN:OD1	1:D:325:LYS:NZ	2.43	0.42
1:B:242:ASP:O	1:B:246:ARG:HB2	2.20	0.42
1:D:250:LEU:HD12	1:D:250:LEU:HA	1.90	0.42
1:B:451:LEU:O	1:B:455:LYS:HG3	2.20	0.41
1:C:391:PRO:HD3	7:C:972:HOH:O	2.19	0.41
1:C:393:ARG:HG2	1:C:404:GLU:CD	2.40	0.41
1:A:392:THR:OG1	1:A:403:LYS:HE2	2.20	0.41
1:B:478:VAL:CG1	1:B:482:SER:HB2	2.50	0.41
1:A:466:ILE:HB	1:A:467:PRO:HD3	2.03	0.41
2:A:751:BOG:H3'2	2:A:752:BOG:H1	2.02	0.41
1:D:450:SER:OG	6:D:604:TRS:H32	2.20	0.41
1:B:87:GLU:CD	1:B:87:GLU:H	2.21	0.41
1:B:59:MET:CE	1:B:318:ILE:HD11	2.51	0.41
1:B:265:GLY:HA3	1:B:290:GLY:CA	2.48	0.41
1:B:406:TRP:NE1	1:B:412:ARG:HD2	2.35	0.41
1:A:335:VAL:O	1:A:339:VAL:HG23	2.20	0.41
1:C:93:VAL:O	1:C:97:LYS:HG2	2.19	0.41
1:D:386:ARG:NH2	6:D:604:TRS:O2	2.49	0.41
1:B:386:ARG:HH22	6:B:603:TRS:C1	2.34	0.41
1:B:325:LYS:NZ	1:C:460:ASN:OD1	2.45	0.41
1:C:13:ASN:HD22	1:C:366:HIS:HE1	1.68	0.41
1:D:314:GLY:HA2	1:D:322:ARG:HH11	1.86	0.41
1:C:245:GLU:C	1:C:248:PRO:HD2	2.41	0.41
1:D:322:ARG:HG2	1:D:327:ILE:O	2.20	0.41
6:D:606:TRS:H21	7:D:930:HOH:O	2.20	0.41
1:D:26:CYS:C	1:D:459:CYS:SG	3.00	0.41
1:A:269:TRP:HA	1:A:269:TRP:CE3	2.56	0.41
1:A:27:ILE:HG12	1:A:30:ASN:ND2	2.35	0.41
1:B:371:LEU:O	1:B:470:GLN:HG2	2.21	0.41
1:A:318:ILE:HG12	1:A:318:ILE:H	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASN:OD1	1:D:310:LYS:HB3	2.20	0.40
1:D:344:LYS:O	1:D:348:GLU:HG3	2.21	0.40
1:C:294:ASP:HA	1:C:337:ASP:OD2	2.21	0.40
1:A:298:PHE:CE1	1:A:309:ILE:HD12	2.56	0.40
1:B:69:ILE:HG23	1:B:232:TYR:CE1	2.57	0.40
1:B:99:PHE:O	1:B:100:LYS:HG3	2.21	0.40
1:C:292:ILE:O	1:C:292:ILE:HD12	2.22	0.40
1:D:388:GLU:HG2	1:D:442:LYS:NZ	2.36	0.40
1:B:65:GLU:CG	1:B:92:MET:HG2	2.50	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	330/376 (88%)	316 (96%)	12 (4%)	2 (1%)	30	29
1	B	326/376 (87%)	308 (94%)	16 (5%)	2 (1%)	30	29
1	C	326/376 (87%)	306 (94%)	18 (6%)	2 (1%)	30	29
1	D	334/376 (89%)	313 (94%)	17 (5%)	4 (1%)	16	12
All	All	1316/1504 (88%)	1243 (94%)	63 (5%)	10 (1%)	24	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	B	291	ASN
1	B	412	ARG
1	C	291	ASN
1	D	291	ASN
1	D	321	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	412	ARG
1	C	412	ARG
1	D	412	ARG
1	D	318	ILE

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	275/308 (89%)	269 (98%)	6 (2%)	60	72
1	B	272/308 (88%)	266 (98%)	6 (2%)	60	72
1	C	272/308 (88%)	265 (97%)	7 (3%)	54	66
1	D	277/308 (90%)	268 (97%)	9 (3%)	46	57
All	All	1096/1232 (89%)	1068 (97%)	28 (3%)	54	66

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	62	VAL
1	A	250	LEU
1	A	266	PHE
1	A	412	ARG
1	A	431	GLU
1	B	33	LEU
1	B	62	VAL
1	B	250	LEU
1	B	266	PHE
1	B	412	ARG
1	B	477	LEU
1	C	33	LEU
1	C	62	VAL
1	C	250	LEU
1	C	266	PHE
1	C	365	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	412	ARG
1	C	477	LEU
1	D	13	ASN
1	D	33	LEU
1	D	62	VAL
1	D	246	ARG
1	D	250	LEU
1	D	266	PHE
1	D	320	ILE
1	D	323	GLU
1	D	412	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	13	ASN
1	A	30	ASN
1	A	44	GLN
1	A	98	ASN
1	A	324	GLN
1	A	331	GLN
1	A	366	HIS
1	B	10	HIS
1	B	13	ASN
1	B	30	ASN
1	B	44	GLN
1	B	331	GLN
1	B	343	ASN
1	B	366	HIS
1	C	10	HIS
1	C	13	ASN
1	C	44	GLN
1	C	331	GLN
1	C	366	HIS
1	D	10	HIS
1	D	13	ASN
1	D	324	GLN
1	D	331	GLN
1	D	366	HIS
1	D	452	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 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$
6	TRS	A	600	3	7,7,7	1.84	2 (28%)	9,9,9	2.62	4 (44%)
6	TRS	A	601	-	7,7,7	1.57	2 (28%)	9,9,9	2.67	4 (44%)
6	TRS	A	607	-	7,7,7	1.70	2 (28%)	9,9,9	2.34	3 (33%)
6	TRS	A	610	-	7,7,7	1.47	1 (14%)	9,9,9	2.65	3 (33%)
2	BOG	A	751	-	20,20,20	1.32	1 (5%)	25,25,25	0.65	0
2	BOG	A	752	-	20,20,20	1.37	2 (10%)	25,25,25	0.65	0
4	IMP	A	801	-	20,25,25	2.57	7 (35%)	22,38,38	3.71	9 (40%)
5	TAD	A	901	-	37,47,47	1.52	8 (21%)	42,72,72	2.95	18 (42%)
6	TRS	B	603	-	7,7,7	1.65	2 (28%)	9,9,9	2.58	2 (22%)
6	TRS	B	608	-	7,7,7	1.63	2 (28%)	9,9,9	2.67	4 (44%)
6	TRS	B	611	-	7,7,7	1.61	2 (28%)	9,9,9	2.57	2 (22%)
4	IMP	B	802	-	20,25,25	2.64	7 (35%)	22,38,38	3.62	9 (40%)
5	TAD	B	902	-	37,47,47	1.56	7 (18%)	42,72,72	2.96	14 (33%)
6	TRS	C	602	-	7,7,7	1.66	2 (28%)	9,9,9	2.51	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TRS	C	605	-	7,7,7	1.67	1 (14%)	9,9,9	2.44	2 (22%)
4	IMP	C	803	-	20,25,25	2.60	6 (30%)	22,38,38	3.61	7 (31%)
5	TAD	C	903	-	37,47,47	1.52	7 (18%)	42,72,72	2.93	15 (35%)
6	TRS	D	604	-	7,7,7	1.65	2 (28%)	9,9,9	2.59	3 (33%)
6	TRS	D	606	-	7,7,7	1.51	1 (14%)	9,9,9	2.69	3 (33%)
6	TRS	D	609	-	7,7,7	1.56	2 (28%)	9,9,9	2.76	4 (44%)
4	IMP	D	804	-	20,25,25	2.49	7 (35%)	22,38,38	3.63	8 (36%)
5	TAD	D	904	-	37,47,47	1.61	7 (18%)	42,72,72	3.56	16 (38%)

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
6	TRS	A	600	3	-	0/9/9/9	0/0/0/0
6	TRS	A	601	-	-	0/9/9/9	0/0/0/0
6	TRS	A	607	-	-	0/9/9/9	0/0/0/0
6	TRS	A	610	-	-	0/9/9/9	0/0/0/0
2	BOG	A	751	-	-	0/11/31/31	0/1/1/1
2	BOG	A	752	-	-	0/11/31/31	0/1/1/1
4	IMP	A	801	-	-	0/6/26/26	0/3/3/3
5	TAD	A	901	-	-	0/18/62/62	0/5/5/5
6	TRS	B	603	-	-	0/9/9/9	0/0/0/0
6	TRS	B	608	-	-	0/9/9/9	0/0/0/0
6	TRS	B	611	-	-	0/9/9/9	0/0/0/0
4	IMP	B	802	-	-	0/6/26/26	0/3/3/3
5	TAD	B	902	-	-	0/18/62/62	0/5/5/5
6	TRS	C	602	-	-	0/9/9/9	0/0/0/0
6	TRS	C	605	-	-	0/9/9/9	0/0/0/0
4	IMP	C	803	-	-	0/6/26/26	0/3/3/3
5	TAD	C	903	-	-	0/18/62/62	0/5/5/5
6	TRS	D	604	-	-	0/9/9/9	0/0/0/0
6	TRS	D	606	-	-	0/9/9/9	0/0/0/0
6	TRS	D	609	-	-	0/9/9/9	0/0/0/0
4	IMP	D	804	-	-	0/6/26/26	0/3/3/3
5	TAD	D	904	-	-	0/18/62/62	0/5/5/5

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	TAD	C2D-C1D	-5.02	1.49	1.53
5	D	904	TAD	C2D-C1D	-4.88	1.49	1.53
5	B	902	TAD	C2D-C1D	-4.87	1.49	1.53
2	A	752	BOG	C3-C2	-4.83	1.39	1.52
5	C	903	TAD	C2D-C1D	-4.81	1.49	1.53
2	A	751	BOG	C3-C2	-4.70	1.40	1.52
6	A	600	TRS	C-N	-3.81	1.45	1.50
4	B	802	IMP	P-O5'	-3.56	1.48	1.60
6	B	608	TRS	C-N	-3.44	1.45	1.50
4	D	804	IMP	P-O5'	-3.38	1.48	1.60
4	A	801	IMP	P-O5'	-3.30	1.49	1.60
6	C	605	TRS	C-N	-3.28	1.45	1.50
4	C	803	IMP	P-O5'	-3.27	1.49	1.60
6	B	611	TRS	C-N	-3.20	1.45	1.50
6	D	604	TRS	C-N	-3.20	1.46	1.50
6	C	602	TRS	C-N	-3.11	1.46	1.50
6	D	606	TRS	C-N	-3.04	1.46	1.50
6	B	603	TRS	C-N	-3.04	1.46	1.50
6	D	609	TRS	C-N	-2.92	1.46	1.50
6	A	610	TRS	C-N	-2.85	1.46	1.50
6	A	607	TRS	C-N	-2.84	1.46	1.50
4	C	803	IMP	C5'-C4'	-2.81	1.42	1.51
5	A	901	TAD	PN-O2N	-2.78	1.49	1.56
4	A	801	IMP	C5'-C4'	-2.65	1.43	1.51
6	A	601	TRS	C-N	-2.63	1.46	1.50
5	D	904	TAD	PN-O2N	-2.53	1.50	1.56
4	D	804	IMP	C5'-C4'	-2.45	1.43	1.51
5	B	902	TAD	PN-O2N	-2.44	1.50	1.56
4	B	802	IMP	C5'-C4'	-2.43	1.43	1.51
5	C	903	TAD	PN-O2N	-2.31	1.50	1.56
5	D	904	TAD	C5A-N7A	-2.24	1.31	1.39
4	B	802	IMP	O2'-C2'	-2.24	1.37	1.43
5	A	901	TAD	C5A-N7A	-2.22	1.31	1.39
5	B	902	TAD	C5A-N7A	-2.18	1.32	1.39
4	A	801	IMP	O2'-C2'	-2.13	1.37	1.43
5	C	903	TAD	C5A-N7A	-2.12	1.32	1.39
4	D	804	IMP	O2'-C2'	-2.07	1.38	1.43
5	A	901	TAD	PA-O2A	-2.03	1.51	1.56
6	B	608	TRS	C3-C	2.03	1.56	1.53
2	A	752	BOG	O1-C1	2.05	1.43	1.40
6	B	611	TRS	C3-C	2.13	1.57	1.53
5	A	901	TAD	C2A-N1A	2.13	1.38	1.33
5	A	901	TAD	O4B-C1B	2.15	1.43	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	TRS	C3-C	2.15	1.57	1.53
5	C	903	TAD	C2A-N1A	2.17	1.38	1.33
5	B	902	TAD	C4A-N3A	2.18	1.38	1.35
6	D	609	TRS	C3-C	2.27	1.57	1.53
6	C	602	TRS	C3-C	2.27	1.57	1.53
5	D	904	TAD	PN-O5D	2.28	1.59	1.57
6	D	604	TRS	C3-C	2.29	1.57	1.53
5	D	904	TAD	C2A-N1A	2.37	1.38	1.33
5	B	902	TAD	O4B-C1B	2.41	1.44	1.41
5	A	901	TAD	PN-O5D	2.43	1.60	1.57
6	A	601	TRS	C3-C	2.43	1.57	1.53
5	D	904	TAD	O4B-C1B	2.44	1.44	1.41
5	C	903	TAD	O4B-C1B	2.44	1.44	1.41
5	C	903	TAD	PA-O5B	2.46	1.60	1.57
5	B	902	TAD	C2A-N1A	2.49	1.38	1.33
6	B	603	TRS	C3-C	2.55	1.57	1.53
5	A	901	TAD	PA-O5B	2.58	1.60	1.57
5	C	903	TAD	PN-O5D	2.59	1.60	1.57
6	A	607	TRS	C3-C	2.88	1.58	1.53
4	D	804	IMP	C6-C5	3.52	1.48	1.41
5	D	904	TAD	PA-O5B	3.75	1.61	1.57
4	A	801	IMP	C6-C5	3.78	1.48	1.41
5	B	902	TAD	PA-O5B	3.89	1.61	1.57
4	C	803	IMP	C6-C5	3.90	1.49	1.41
4	B	802	IMP	C6-C5	3.97	1.49	1.41
4	D	804	IMP	C8-N7	4.52	1.43	1.34
4	C	803	IMP	C8-N7	4.57	1.43	1.34
4	B	802	IMP	C8-N7	4.66	1.43	1.34
4	A	801	IMP	C8-N7	4.78	1.43	1.34
4	D	804	IMP	C6-N1	5.02	1.42	1.33
4	D	804	IMP	C2-N1	5.12	1.43	1.33
4	A	801	IMP	C2-N1	5.12	1.43	1.33
4	A	801	IMP	C6-N1	5.44	1.43	1.33
4	B	802	IMP	C2-N1	5.46	1.44	1.33
4	C	803	IMP	C6-N1	5.48	1.43	1.33
4	B	802	IMP	C6-N1	5.50	1.43	1.33
4	C	803	IMP	C2-N1	5.55	1.44	1.33

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	IMP	N3-C2-N1	-12.85	119.06	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	802	IMP	N3-C2-N1	-12.57	119.27	128.89
4	C	803	IMP	N3-C2-N1	-12.46	119.36	128.89
4	D	804	IMP	N3-C2-N1	-12.39	119.41	128.89
5	B	902	TAD	N3A-C2A-N1A	-12.16	119.59	128.89
5	D	904	TAD	N3A-C2A-N1A	-12.10	119.63	128.89
5	A	901	TAD	N3A-C2A-N1A	-11.85	119.82	128.89
5	C	903	TAD	N3A-C2A-N1A	-11.82	119.84	128.89
5	D	904	TAD	C4N-C6N-N6N	-8.89	107.49	116.21
5	B	902	TAD	C4N-C6N-N6N	-3.75	112.53	116.21
5	D	904	TAD	O1N-PN-C3	-3.63	99.89	109.02
5	B	902	TAD	O1N-PN-C3	-3.60	99.95	109.02
5	C	903	TAD	O1N-PN-C3	-3.59	99.98	109.02
5	C	903	TAD	C4N-C6N-N6N	-3.47	112.81	116.21
5	A	901	TAD	O1N-PN-C3	-3.47	100.30	109.02
6	B	603	TRS	C1-C-N	-3.40	101.90	108.09
6	C	605	TRS	C1-C-N	-3.35	102.00	108.09
6	B	611	TRS	C1-C-N	-3.34	102.01	108.09
6	C	602	TRS	C1-C-N	-3.34	102.01	108.09
5	A	901	TAD	C4N-C6N-N6N	-3.31	112.97	116.21
6	D	609	TRS	C1-C-N	-3.19	102.28	108.09
6	D	604	TRS	C1-C-N	-3.09	102.45	108.09
6	A	600	TRS	C1-C-N	-2.96	102.70	108.09
6	A	607	TRS	C1-C-N	-2.88	102.86	108.09
4	C	803	IMP	C1'-N9-C4	-2.87	122.61	126.94
6	D	606	TRS	C1-C-N	-2.87	102.87	108.09
4	A	801	IMP	C1'-N9-C4	-2.80	122.71	126.94
6	A	601	TRS	C1-C-N	-2.70	103.17	108.09
4	B	802	IMP	C1'-N9-C4	-2.67	122.91	126.94
6	A	610	TRS	C2-C-C1	-2.65	105.05	110.78
6	B	608	TRS	C1-C-N	-2.63	103.30	108.09
4	D	804	IMP	C1'-N9-C4	-2.51	123.15	126.94
6	A	610	TRS	C1-C-N	-2.45	103.62	108.09
5	A	901	TAD	C1B-N9A-C4A	-2.42	123.30	126.94
5	C	903	TAD	C1B-N9A-C4A	-2.41	123.30	126.94
5	C	903	TAD	C5D-C4D-C3D	-2.39	105.73	115.21
6	A	601	TRS	C2-C-C1	-2.33	105.73	110.78
6	D	609	TRS	C2-C-C1	-2.32	105.76	110.78
6	A	601	TRS	C3-C-C2	-2.30	105.81	110.78
6	B	608	TRS	C3-C-C2	-2.28	105.84	110.78
5	A	901	TAD	O5D-PN-O1N	-2.28	107.92	113.98
6	D	604	TRS	C3-C-C2	-2.22	105.98	110.78
6	A	607	TRS	C2-C-C1	-2.21	105.99	110.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	TAD	C5D-C4D-C3D	-2.14	106.71	115.21
5	A	901	TAD	C4D-O4D-C1D	-2.14	107.39	109.58
6	D	606	TRS	C3-C-C2	-2.13	106.17	110.78
6	A	600	TRS	C3-C-C2	-2.11	106.20	110.78
6	C	602	TRS	C3-C-C2	-2.10	106.23	110.78
6	B	608	TRS	C2-C-C1	-2.08	106.28	110.78
5	D	904	TAD	C5D-C4D-C3D	-2.05	107.06	115.21
6	D	609	TRS	C3-C-C2	-2.04	106.37	110.78
5	B	902	TAD	C5D-C4D-C3D	-2.03	107.16	115.21
5	D	904	TAD	O5D-PN-O1N	-2.01	108.64	113.98
5	A	901	TAD	O1A-PA-C3	2.01	114.09	109.02
4	A	801	IMP	O3P-P-O5'	2.02	112.37	106.56
4	B	802	IMP	O3P-P-O5'	2.04	112.45	106.56
6	A	600	TRS	C3-C-C1	2.07	115.26	110.78
4	B	802	IMP	C4'-O4'-C1'	2.08	112.01	109.72
5	C	903	TAD	O4D-C4D-C5D	2.08	116.78	109.32
5	A	901	TAD	O4D-C4D-C5D	2.09	116.81	109.32
4	D	804	IMP	O3P-P-O5'	2.11	112.64	106.56
5	B	902	TAD	C3D-C2D-C1D	2.18	104.32	101.79
5	D	904	TAD	C3D-C2D-C1D	2.19	104.33	101.79
4	A	801	IMP	C4'-O4'-C1'	2.21	112.15	109.72
5	A	901	TAD	O2N-PN-O1N	2.34	117.49	110.12
5	C	903	TAD	O2N-PN-O1N	2.39	117.62	110.12
5	D	904	TAD	O4D-C4D-C5D	2.40	117.92	109.32
5	D	904	TAD	C2A-N1A-C6A	2.46	123.16	118.77
4	C	803	IMP	C5'-C4'-C3'	2.49	125.08	115.21
5	B	902	TAD	C2A-N1A-C6A	2.50	123.23	118.77
5	B	902	TAD	O2N-PN-O1N	2.52	118.05	110.12
5	A	901	TAD	C2A-N1A-C6A	2.58	123.38	118.77
5	C	903	TAD	C2A-N1A-C6A	2.59	123.40	118.77
4	D	804	IMP	C5'-C4'-C3'	2.59	125.50	115.21
5	D	904	TAD	C2D-C3D-C4D	2.59	107.94	102.61
5	C	903	TAD	C4B-O4B-C1B	2.60	112.58	109.72
4	A	801	IMP	C5'-C4'-C3'	2.60	125.55	115.21
5	B	902	TAD	C2D-C3D-C4D	2.63	108.01	102.61
5	D	904	TAD	O2N-PN-O1N	2.64	118.43	110.12
4	B	802	IMP	C5'-C4'-C3'	2.70	125.92	115.21
5	C	903	TAD	C2D-C3D-C4D	2.70	108.16	102.61
5	C	903	TAD	C2B-C3B-C4B	2.71	108.18	102.61
5	A	901	TAD	C2D-C3D-C4D	2.80	108.36	102.61
5	A	901	TAD	C2B-C3B-C4B	2.86	108.49	102.61
5	D	904	TAD	C2B-C3B-C4B	2.96	108.70	102.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	TAD	C2B-C3B-C4B	3.02	108.83	102.61
5	A	901	TAD	C4B-O4B-C1B	3.10	113.12	109.72
4	C	803	IMP	O3'-C3'-C4'	3.24	120.76	111.05
4	B	802	IMP	C4-C5-N7	3.25	112.47	109.48
4	B	802	IMP	O3'-C3'-C4'	3.26	120.83	111.05
4	A	801	IMP	O3'-C3'-C4'	3.28	120.89	111.05
4	A	801	IMP	C4-C5-N7	3.33	112.54	109.48
4	C	803	IMP	C4-C5-N7	3.34	112.55	109.48
4	D	804	IMP	C4-C5-N7	3.39	112.60	109.48
4	D	804	IMP	O3'-C3'-C4'	3.41	121.27	111.05
5	B	902	TAD	C4B-O4B-C1B	3.52	113.59	109.72
5	D	904	TAD	C4B-O4B-C1B	3.82	113.91	109.72
5	C	903	TAD	O4B-C4B-C5B	4.05	123.79	109.32
5	A	901	TAD	O4B-C4B-C5B	4.18	124.27	109.32
5	C	903	TAD	C4A-C5A-N7A	4.39	113.52	109.48
5	D	904	TAD	O4B-C4B-C5B	4.41	125.10	109.32
5	B	902	TAD	O4B-C4B-C5B	4.49	125.39	109.32
5	A	901	TAD	C4A-C5A-N7A	4.60	113.71	109.48
5	A	901	TAD	O6N-C6N-C4N	4.74	124.04	119.67
5	D	904	TAD	C4A-C5A-N7A	4.76	113.85	109.48
5	B	902	TAD	C4A-C5A-N7A	4.79	113.89	109.48
5	B	902	TAD	O6N-C6N-C4N	5.03	124.31	119.67
5	C	903	TAD	O6N-C6N-C4N	5.21	124.48	119.67
4	C	803	IMP	O4'-C1'-N9	5.34	119.29	108.10
4	B	802	IMP	O4'-C1'-N9	5.37	119.34	108.10
4	D	804	IMP	O4'-C1'-N9	5.44	119.49	108.10
6	A	607	TRS	C2-C-N	5.63	118.34	108.09
6	C	605	TRS	C2-C-N	5.73	118.51	108.09
4	A	801	IMP	O4'-C1'-N9	5.76	120.16	108.10
6	C	602	TRS	C2-C-N	5.85	118.74	108.09
6	D	604	TRS	C2-C-N	5.90	118.82	108.09
5	B	902	TAD	O4D-C1D-C2D	5.94	110.79	104.73
6	B	603	TRS	C2-C-N	5.98	118.97	108.09
6	B	611	TRS	C2-C-N	6.09	119.18	108.09
6	B	608	TRS	C2-C-N	6.15	119.28	108.09
6	A	600	TRS	C2-C-N	6.19	119.35	108.09
6	A	601	TRS	C2-C-N	6.29	119.54	108.09
6	D	606	TRS	C2-C-N	6.31	119.56	108.09
6	A	610	TRS	C2-C-N	6.31	119.57	108.09
6	D	609	TRS	C2-C-N	6.47	119.86	108.09
5	D	904	TAD	O4D-C1D-C2D	6.54	111.40	104.73
5	C	903	TAD	O4D-C1D-C2D	6.64	111.50	104.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	TAD	O4D-C1D-C2D	6.89	111.76	104.73
4	B	802	IMP	C2-N1-C6	7.01	126.67	116.04
4	C	803	IMP	C2-N1-C6	7.07	126.76	116.04
4	A	801	IMP	C2-N1-C6	7.12	126.83	116.04
4	D	804	IMP	C2-N1-C6	7.18	126.92	116.04
5	D	904	TAD	O6N-C6N-C4N	10.74	129.57	119.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	TRS	1	0
6	A	601	TRS	1	0
6	A	607	TRS	2	0
6	A	610	TRS	1	0
2	A	751	BOG	1	0
2	A	752	BOG	2	0
6	B	603	TRS	1	0
6	B	608	TRS	1	0
5	B	902	TAD	1	0
6	C	605	TRS	4	0
6	D	604	TRS	2	0
6	D	606	TRS	2	0
6	D	609	TRS	3	0
4	D	804	IMP	2	0
5	D	904	TAD	3	0

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.