



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 01:17 AM EDT

PDB ID : 3TOX
Title : Crystal structure of a short chain dehydrogenase in complex with NAD(P) from *Sinorhizobium meliloti* 1021
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on : unknown
Resolution : 1.93 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

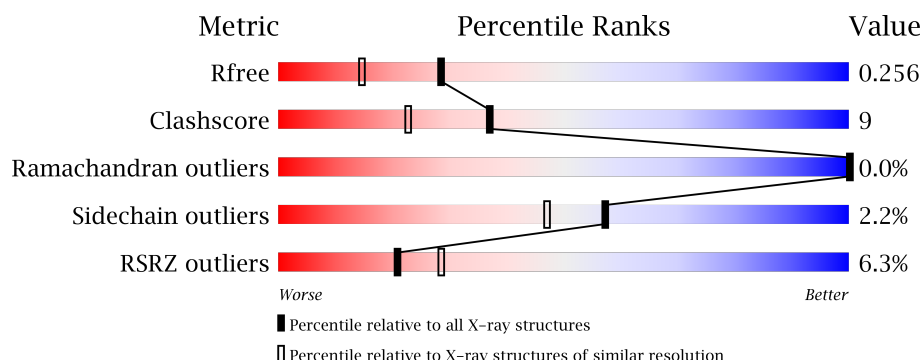
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.93 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}	100719	3233 (1.96-1.92)
Clashscore	112137	3430 (1.96-1.92)
Ramachandran outliers	110173	3395 (1.96-1.92)
Sidechain outliers	110143	3395 (1.96-1.92)
RSRZ outliers	101464	3250 (1.96-1.92)

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	280	<div> <div>4%</div> <div>79%</div> <div>11%</div> <div>9%</div> </div>
1	B	280	<div> <div>7%</div> <div>75%</div> <div>13%</div> <div>11%</div> </div>
1	C	280	<div> <div>4%</div> <div>81%</div> <div>9%</div> <div>9%</div> </div>
1	D	280	<div> <div>4%</div> <div>80%</div> <div>10%</div> <div>9%</div> </div>
1	E	280	<div> <div>8%</div> <div>71%</div> <div>18%</div> <div>9%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	280	<div><div>8%</div><div><div></div><div>78%</div><div>11%</div><div>•</div><div>9%</div></div></div>
1	G	280	<div><div>8%</div><div><div></div><div>75%</div><div>14%</div><div>•</div><div>10%</div></div></div>
1	I	280	<div><div>4%</div><div><div></div><div>75%</div><div>14%</div><div>••</div><div>9%</div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15313 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 Short chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			
1	B	248	Total	C	N	O	S	0	0	0
			1725	1080	306	338	1			
1	C	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			
1	D	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			
1	E	254	Total	C	N	O	S	0	0	0
			1764	1105	312	346	1			
1	F	254	Total	C	N	O	S	0	0	0
			1761	1102	312	346	1			
1	G	251	Total	C	N	O	S	0	0	0
			1745	1094	309	341	1			
1	I	254	Total	C	N	O	S	0	0	0
			1771	1112	312	346	1			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q92SS3
A	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
A	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
A	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
A	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
A	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
A	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
A	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
A	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
A	266	SER	-	EXPRESSION TAG	UNP Q92SS3
A	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
A	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
A	269	HIS	-	EXPRESSION TAG	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
A	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
A	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
A	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
A	274	SER	-	EXPRESSION TAG	UNP Q92SS3
A	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
A	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
A	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
A	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
A	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
A	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
B	1	MET	-	EXPRESSION TAG	UNP Q92SS3
B	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
B	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
B	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
B	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
B	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
B	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
B	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
B	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
B	266	SER	-	EXPRESSION TAG	UNP Q92SS3
B	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	269	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
B	274	SER	-	EXPRESSION TAG	UNP Q92SS3
B	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
B	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
B	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
B	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
B	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
B	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
C	1	MET	-	EXPRESSION TAG	UNP Q92SS3
C	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
C	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
C	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
C	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
C	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
C	263	TYR	-	EXPRESSION TAG	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
C	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
C	266	SER	-	EXPRESSION TAG	UNP Q92SS3
C	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	269	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
C	274	SER	-	EXPRESSION TAG	UNP Q92SS3
C	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
C	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
C	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
C	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
C	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
C	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
D	1	MET	-	EXPRESSION TAG	UNP Q92SS3
D	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
D	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
D	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
D	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
D	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
D	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
D	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
D	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
D	266	SER	-	EXPRESSION TAG	UNP Q92SS3
D	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	269	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
D	274	SER	-	EXPRESSION TAG	UNP Q92SS3
D	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
D	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
D	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
D	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
D	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
D	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
E	1	MET	-	EXPRESSION TAG	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
E	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
E	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
E	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
E	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
E	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
E	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
E	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
E	266	SER	-	EXPRESSION TAG	UNP Q92SS3
E	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	269	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
E	274	SER	-	EXPRESSION TAG	UNP Q92SS3
E	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
E	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
E	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
E	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
E	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
E	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
F	1	MET	-	EXPRESSION TAG	UNP Q92SS3
F	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
F	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
F	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
F	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
F	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
F	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
F	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
F	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
F	266	SER	-	EXPRESSION TAG	UNP Q92SS3
F	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
F	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
F	269	HIS	-	EXPRESSION TAG	UNP Q92SS3
F	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
F	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
F	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
F	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
F	274	SER	-	EXPRESSION TAG	UNP Q92SS3
F	275	HIS	-	EXPRESSION TAG	UNP Q92SS3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
F	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
F	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
F	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
F	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
G	1	MET	-	EXPRESSION TAG	UNP Q92SS3
G	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
G	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
G	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
G	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
G	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
G	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
G	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
G	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
G	266	SER	-	EXPRESSION TAG	UNP Q92SS3
G	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	269	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
G	274	SER	-	EXPRESSION TAG	UNP Q92SS3
G	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
G	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
G	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
G	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
G	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
G	280	LYS	-	EXPRESSION TAG	UNP Q92SS3
I	1	MET	-	EXPRESSION TAG	UNP Q92SS3
I	2	VAL	-	EXPRESSION TAG	UNP Q92SS3
I	259	ALA	-	EXPRESSION TAG	UNP Q92SS3
I	260	GLU	-	EXPRESSION TAG	UNP Q92SS3
I	261	ASN	-	EXPRESSION TAG	UNP Q92SS3
I	262	LEU	-	EXPRESSION TAG	UNP Q92SS3
I	263	TYR	-	EXPRESSION TAG	UNP Q92SS3
I	264	PHE	-	EXPRESSION TAG	UNP Q92SS3
I	265	GLN	-	EXPRESSION TAG	UNP Q92SS3
I	266	SER	-	EXPRESSION TAG	UNP Q92SS3
I	267	HIS	-	EXPRESSION TAG	UNP Q92SS3
I	268	HIS	-	EXPRESSION TAG	UNP Q92SS3
I	269	HIS	-	EXPRESSION TAG	UNP Q92SS3

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	270	HIS	-	EXPRESSION TAG	UNP Q92SS3
I	271	HIS	-	EXPRESSION TAG	UNP Q92SS3
I	272	HIS	-	EXPRESSION TAG	UNP Q92SS3
I	273	TRP	-	EXPRESSION TAG	UNP Q92SS3
I	274	SER	-	EXPRESSION TAG	UNP Q92SS3
I	275	HIS	-	EXPRESSION TAG	UNP Q92SS3
I	276	PRO	-	EXPRESSION TAG	UNP Q92SS3
I	277	GLN	-	EXPRESSION TAG	UNP Q92SS3
I	278	PHE	-	EXPRESSION TAG	UNP Q92SS3
I	279	GLU	-	EXPRESSION TAG	UNP Q92SS3
I	280	LYS	-	EXPRESSION TAG	UNP Q92SS3

- # NAP
-
- The chemical structure of Naproxen (NAP) is shown, featuring a naphthalene ring system. The structure includes a carboxylic acid group (-COOH) at the 2-position, a chiral center at the 1-position, and a 6-methoxy group (-OCH₃). The stereochemistry is indicated by wedged and dashed bonds. The structure is labeled with various atoms and groups, including N1A, N1B, N1C, N1D, N1E, N1F, N1G, N1H, N1I, N1J, N1K, N1L, N1M, N1N, N1O, N1P, N1Q, N1R, N1S, N1T, N1U, N1V, N1W, N1X, N1Y, N1Z, N1AA, N1AB, N1AC, N1AD, N1AE, N1AF, N1AG, N1AH, N1AI, N1AJ, N1AK, N1AL, N1AM, N1AN, N1AO, N1AP, N1AQ, N1AR, N1AS, N1AT, N1AU, N1AV, N1AW, N1AX, N1AY, N1AZ, N1BA, N1BB, N1BC, N1BD, N1BE, N1BF, N1BG, N1BH, N1BI, N1BJ, N1BK, N1BL, N1BM, N1BN, N1BO, N1BP, N1BQ, N1BR, N1BS, N1BT, N1BU, N1BV, N1BW, N1BX, N1BY, N1BZ, N1CA, N1CB, N1CC, N1CD, N1CE, N1CF, N1CG, N1CH, N1CI, N1CJ, N1CK, N1CL, N1CM, N1CN, N1CO, N1CP, N1CQ, N1CR, N1CS, N1CT, N1CU, N1CV, N1CW, N1CX, N1CY, N1CZ, N1DA, N1DB, N1DC, N1DD, N1DE, N1DF, N1DG, N1DH, N1DI, N1DJ, N1DK, N1DL, N1DM, N1DN, N1DO, N1DP, N1DQ, N1DR, N1DS, N1DT, N1DU, N1DV, N1DW, N1DX, N1DY, N1DZ, N1EA, N1EB, N1EC, N1ED, N1EE, N1EF, N1EG, N1EH, N1EI, N1EJ, N1EK, N1EL, N1EM, N1EN, N1EO, N1EP, N1EQ, N1ER, N1ES, N1ET, N1EU, N1EV, N1EW, N1EX, N1EY, N1EZ, N1FA, N1FB, N1FC, N1FD, N1FE, N1FF, N1FG, N1FH, N1FI, N1FJ, N1FK, N1FL, N1FM, N1FN, N1FO, N1FP, N1FQ, N1FR, N1FS, N1FT, N1FU, N1FV, N1FW, N1FX, N1FY, N1FZ, N1GA, N1GB, N1GC, N1GD, N1GE, N1GF, N1GG, N1GH, N1GI, N1GJ, N1GK, N1GL, N1GM, N1GN, N1GO, N1GP, N1GQ, N1GR, N1GS, N1GT, N1GU, N1GV, N1GW, N1GX, N1GY, N1GZ, N1HA, N1HB, N1HC, N1HD, N1HE, N1HF, N1HG, N1HH, N1HI, N1HJ, N1HK, N1HL, N1HM, N1HN, N1HO, N1HP, N1HQ, N1HR, N1HS, N1HT, N1HU, N1HV, N1HW, N1HX, N1HY, N1HZ, N1IA, N1IB, N1IC, N1ID, N1IE, N1IF, N1IG, N1IH, N1II, N1IJ, N1IK, N1IL, N1IM, N1IN, N1IO, N1IP, N1IQ, N1IR, N1IS, N1IT, N1IU, N1IV, N1IW, N1IX, N1IY, N1IZ, N1JA, N1JB, N1JC, N1JD, N1JE, N1JF, N1JG, N1JH, N1JI, N1JJ, N1JK, N1JL, N1JM, N1JN, N1JO, N1JP, N1JQ, N1JR, N1JS, N1JT, N1JU, N1JV, N1JW, N1JX, N1JY, N1JZ, N1KA, N1KB, N1KC, N1KD, N1KE, N1KF, N1KG, N1KH, N1KI, N1KJ, N1KK, N1KL, N1KM, N1KN, N1KO, N1KP, N1KQ, N1KR, N1KS, N1KT, N1KU, N1KV, N1KW, N1KX, N1KY, N1KZ, N1LA, N1LB, N1LC, N1LD, N1LE, N1LF, N1LG, N1LH, N1LI, N1LJ, N1LK, N1LL, N1LM, N1LN, N1LO, N1LP, N1LQ, N1LR, N1LS, N1LT, N1LU, N1LV, N1LW, N1LX, N1LY, N1LZ, N1MA, N1MB, N1MC, N1MD, N1ME, N1MF, N1MG, N1MH, N1MI, N1MJ, N1MK, N1ML, N1MM, N1MN, N1MO, N1MP, N1MQ, N1MR, N1MS, N1MT, N1MU, N1MV, N1MW, N1MX, N1MY, N1MZ, N1NA, N1NB, N1NC, N1ND, N1NE, N1NF, N1NG, N1NH, N1NI, N1NJ, N1NK, N1NL, N1NM, N1NN, N1NO, N1NP, N1NQ, N1NR, N1NS, N1NT, N1NU, N1NV, N1NW, N1NX, N1NY, N1NZ, N1OA, N1OB, N1OC, N1OD, N1OE, N1OF, N1OG, N1OH, N1OI, N1OJ, N1OK, N1OL, N1OM, N1ON, N1OO, N1OP, N1OQ, N1OR, N1OS, N1OT, N1OU, N1OV, N1OW, N1OX, N1OY, N1OZ, N1PA, N1PB, N1PC, N1PD, N1PE, N1PF, N1PG, N1PH, N1PI, N1PJ, N1PK, N1PL, N1PM, N1PN, N1PO, N1PP, N1PQ, N1PR, N1PS, N1PT, N1PU, N1PV, N1PW, N1PX, N1PY, N1PZ, N1QA, N1QB, N1QC, N1QD, N1QE, N1QF, N1QG, N1QH, N1QI, N1QJ, N1QK, N1QL, N1QM, N1QN, N1QO, N1QP, N1QQ, N1QR, N1QS, N1QT, N1QU, N1QV, N1QW, N1QX, N1QY, N1QZ, N1RA, N1RB, N1RC, N1RD, N1RE, N1RF, N1RG, N1RH, N1RI, N1RJ, N1RK, N1RL, N1RM, N1RN, N1RO, N1RP, N1RQ, N1RR, N1RS, N1RT, N1RU, N1RV, N1RW, N1RX, N1RY, N1RZ, N1SA, N1SB, N1SC, N1SD, N1SE, N1SF, N1SG, N1SH, N1SI, N1SJ, N1SK, N1SL, N1SM, N1SN, N1SO, N1SP, N1SQ, N1SR, N1SS, N1ST, N1SU, N1SV, N1SW, N1SX, N1SY, N1SZ, N1TA, N1TB, N1TC, N1TD, N1TE, N1TF, N1TG, N1TH, N1TI, N1TJ, N1TK, N1TL, N1TM, N1TN, N1TO, N1TP, N1TQ, N1TR, N1TS, N1TT, N1TU, N1TV, N1TW, N1TX, N1TY, N1TZ, N1UA, N1UB, N1UC, N1UD, N1UE, N1UF, N1UG, N1UH, N1UI, N1UJ, N1UK, N1UL, N1UM, N1UN, N1UO, N1UP, N1UQ, N1UR, N1US, N1UT, N1UU, N1UV, N1UW, N1UX, N1UY, N1UZ, N1VA, N1VB, N1VC, N1VD, N1VE, N1VF, N1VG, N1VH, N1VI, N1VJ, N1VK, N1VL, N1VM, N1VN, N1VO, N1VP, N1VQ, N1VR, N1VS, N1VT, N1VU, N1VV, N1VW, N1VX, N1VY, N1VZ, N1WA, N1WB, N1WC, N1WD, N1WE, N1WF, N1WG, N1WH, N1WI, N1WJ, N1WK, N1WL, N1WM, N1WN, N1WO, N1WP, N1WQ, N1WR, N1WS, N1WT, N1WU, N1WV, N1WW, N1WX, N1WY, N1WZ, N1XA, N1XB, N1XC, N1XD, N1XE, N1XF, N1XG, N1XH, N1XI, N1XJ, N1XK, N1XL, N1XM, N1XN, N1XO, N1XP, N1XQ, N1XR, N1XS, N1XT, N1XU, N1XV, N1XW, N1XX, N1XY, N1XZ, N1YA, N1YB, N1YC, N1YD, N1YE, N1YF, N1YG, N1YH, N1YI, N1YJ, N1YK, N1YL, N1YM, N1YN, N1YO, N1YP, N1YQ, N1YR, N1YS, N1YT, N1YU, N1YV, N1YW, N1YX, N1YY, N1YZ, N1ZA, N1ZB, N1ZC, N1ZD, N1ZE, N1ZF, N1ZG, N1ZH, N1ZI, N1ZJ, N1ZK, N1ZL, N1ZM, N1ZN, N1ZO, N1ZP, N1ZQ, N1ZR, N1ZS, N1ZT, N1ZU, N1ZV, N1ZW, N1ZX, N1ZY, N1ZZ.

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



Continued from previous page...

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

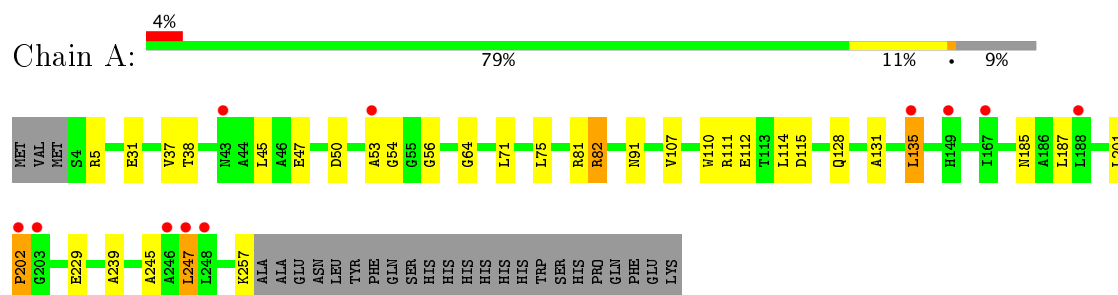
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	82	Total	O	0	0
			82	82		
3	C	130	Total	O	0	0
			130	130		
3	D	117	Total	O	0	0
			117	117		
3	E	96	Total	O	0	0
			96	96		
3	F	79	Total	O	0	0
			79	79		
3	G	92	Total	O	0	0
			92	92		
3	I	132	Total	O	0	0
			132	132		

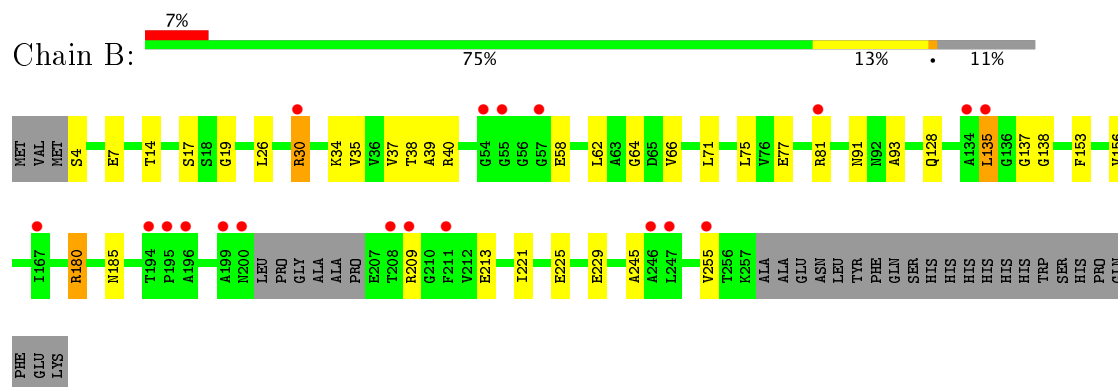
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

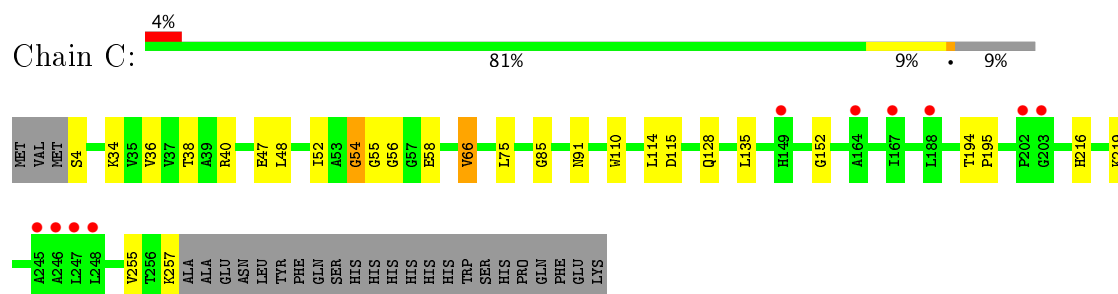
- Molecule 1: Short chain dehydrogenase



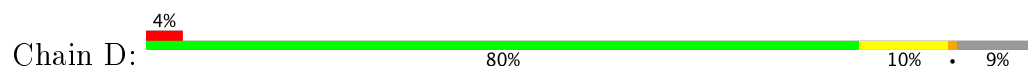
- Molecule 1: Short chain dehydrogenase

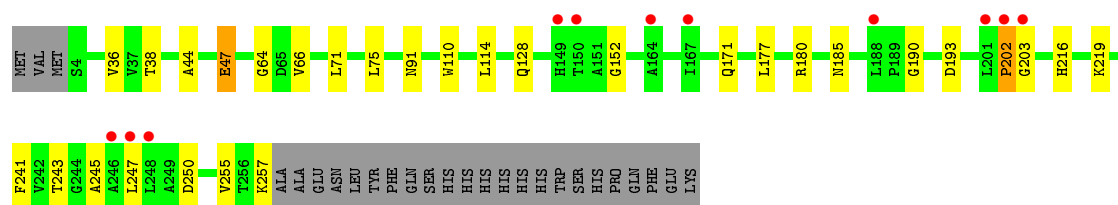


- Molecule 1: Short chain dehydrogenase

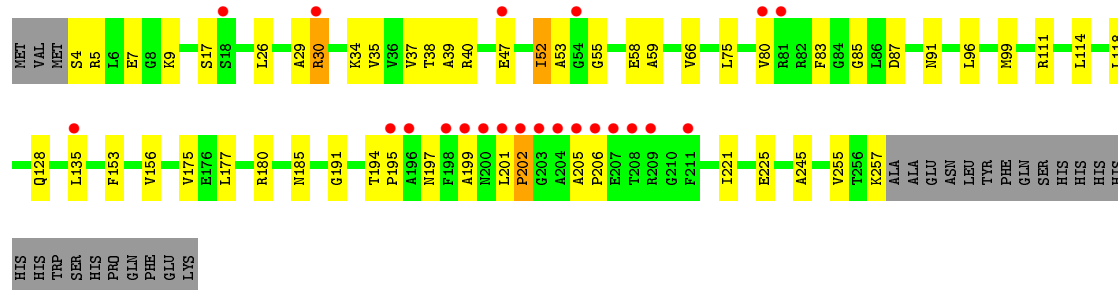


- Molecule 1: Short chain dehydrogenase

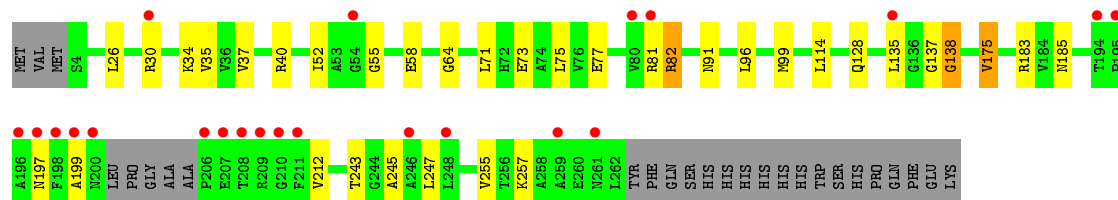
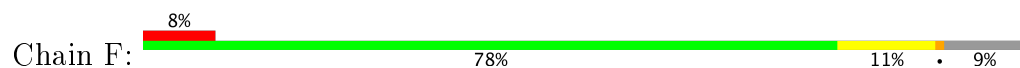




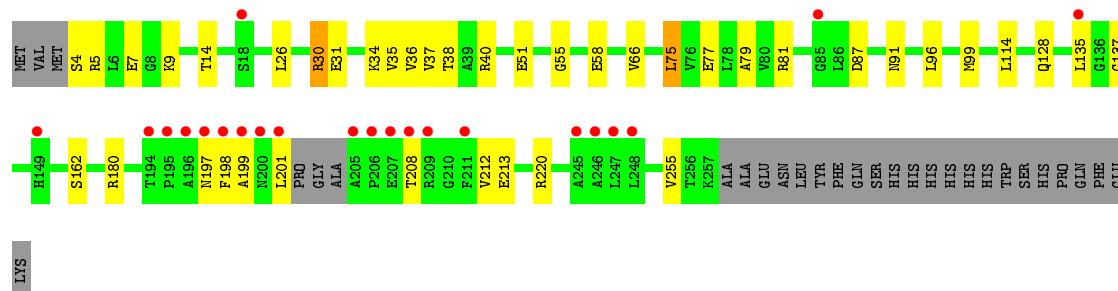
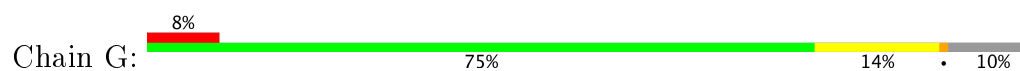
• Molecule 1: Short chain dehydrogenase



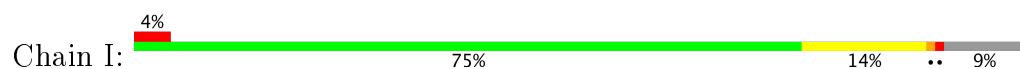
• Molecule 1: Short chain dehydrogenase

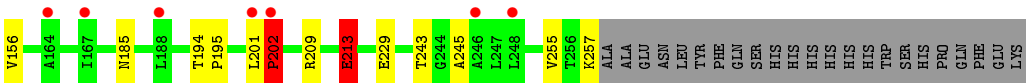


• Molecule 1: Short chain dehydrogenase



• Molecule 1: Short chain dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.97Å 122.94Å 139.82Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	43.47 – 1.93 43.47 – 1.93	Depositor EDS
% Data completeness (in resolution range)	87.4 (43.47-1.93) 87.4 (43.47-1.93)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.200 , 0.255 0.203 , 0.256	Depositor DCC
R_{free} test set	6812 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.417 for k,h,-l 0.387 for -k,-h,-l 0.399 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15313	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	1.15	1/1795 (0.1%)	0.94	4/2437 (0.2%)
1	B	1.08	3/1745 (0.2%)	0.92	2/2366 (0.1%)
1	C	1.16	1/1795 (0.1%)	0.95	2/2437 (0.1%)
1	D	1.17	1/1795 (0.1%)	0.95	0/2437
1	E	1.03	2/1787 (0.1%)	0.92	3/2426 (0.1%)
1	F	1.06	2/1782 (0.1%)	0.91	1/2417 (0.0%)
1	G	1.05	0/1766	0.86	1/2396 (0.0%)
1	I	1.19	4/1795 (0.2%)	0.96	1/2437 (0.0%)
All	All	1.11	14/14260 (0.1%)	0.93	14/19353 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	G	0	1
1	I	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	255	VAL	CB-CG2	-5.89	1.40	1.52
1	I	213	GLU	CG-CD	-5.89	1.43	1.51
1	F	138	GLY	N-CA	-5.88	1.37	1.46
1	E	175	VAL	CB-CG1	5.83	1.65	1.52
1	F	175	VAL	CB-CG1	5.80	1.65	1.52
1	E	225	GLU	CB-CG	5.68	1.62	1.52
1	B	229	GLU	CB-CG	5.49	1.62	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	76	VAL	CB-CG2	5.48	1.64	1.52
1	A	239	ALA	CA-CB	5.42	1.63	1.52
1	I	255	VAL	CB-CG2	-5.34	1.41	1.52
1	B	137	GLY	C-O	-5.30	1.15	1.23
1	I	133	ALA	CA-CB	-5.11	1.41	1.52
1	D	241	PHE	CE2-CZ	5.08	1.47	1.37
1	B	225	GLU	CB-CG	5.01	1.61	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	GLY	N-CA-C	5.84	127.71	113.10
1	A	202	PRO	CA-C-N	5.74	127.67	116.20
1	C	55	GLY	N-CA-C	-5.74	98.76	113.10
1	I	30	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	115	ASP	CB-CG-OD1	5.51	123.25	118.30
1	A	202	PRO	N-CA-C	5.46	126.29	112.10
1	B	62	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	247	LEU	CB-CG-CD2	5.33	120.05	111.00
1	E	5	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	A	115	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	180	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	E	30	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	F	183	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	E	202	PRO	N-CA-C	5.07	125.29	112.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	54	GLY	Peptide
1	G	137	GLY	Peptide
1	I	202	PRO	Peptide

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	1771	0	1774	29	0
1	B	1725	0	1724	26	0
1	C	1771	0	1774	23	0
1	D	1771	0	1774	30	0
1	E	1764	0	1763	47	0
1	F	1761	0	1752	37	0
1	G	1745	0	1747	35	0
1	I	1771	0	1774	39	0
2	A	48	0	25	0	0
2	B	48	0	25	1	0
2	C	48	0	25	2	0
2	D	48	0	25	1	0
2	E	48	0	25	4	0
2	F	48	0	25	2	0
2	G	48	0	25	3	0
2	I	48	0	25	0	0
3	A	122	0	0	3	0
3	B	82	0	0	2	0
3	C	130	0	0	3	0
3	D	117	0	0	1	0
3	E	96	0	0	5	0
3	F	79	0	0	2	0
3	G	92	0	0	1	0
3	I	132	0	0	3	0
All	All	15313	0	14282	255	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 9.

All (255) 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:F:96:LEU:HB3	1:F:99:MET:HE3	1.31	1.10
1:G:96:LEU:HB3	1:G:99:MET:HE3	1.34	1.09
1:G:198:PHE:HA	1:G:201:LEU:HD13	1.30	1.06
1:I:135:LEU:N	1:I:135:LEU:CD1	2.18	1.05
1:G:198:PHE:HA	1:G:201:LEU:CD1	1.87	1.04
1:B:180:ARG:HH11	1:B:180:ARG:HG3	1.24	1.01
1:I:44:ALA:O	1:I:47:GLU:HG3	1.62	0.97
1:I:135:LEU:H	1:I:135:LEU:HD13	1.32	0.95
1:E:99:MET:HE2	1:E:156:VAL:HG12	1.47	0.94
1:I:135:LEU:N	1:I:135:LEU:HD13	1.84	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:99:MET:CE	1:E:156:VAL:HG12	2.07	0.84
1:I:135:LEU:N	1:I:135:LEU:HD12	1.94	0.82
1:I:99:MET:CE	1:I:156:VAL:HG12	2.11	0.81
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.43	0.81
1:I:99:MET:HE1	1:I:156:VAL:HG12	1.61	0.81
1:A:131:ALA:O	1:A:135:LEU:HD23	1.80	0.81
1:I:86:LEU:H	1:I:135:LEU:HD21	1.45	0.80
1:D:202:PRO:O	1:D:202:PRO:CG	2.30	0.80
1:D:202:PRO:O	1:D:202:PRO:CD	2.29	0.78
1:E:30:ARG:CZ	3:E:711:HOH:O	2.30	0.78
1:E:4:SER:HB2	1:E:7:GLU:HB2	1.66	0.77
1:G:30:ARG:HD3	1:G:30:ARG:N	1.96	0.77
1:A:91:ASN:HD21	1:A:128:GLN:HE22	1.34	0.76
1:E:40:ARG:HD3	3:E:794:HOH:O	1.85	0.76
1:E:91:ASN:HD21	1:E:128:GLN:HE22	1.36	0.74
1:G:91:ASN:HD21	1:G:128:GLN:HE22	1.36	0.73
1:G:198:PHE:CA	1:G:201:LEU:CD1	2.65	0.73
1:F:26:LEU:HD23	1:F:52:ILE:CD1	2.18	0.73
1:I:91:ASN:HD21	1:I:128:GLN:HE22	1.34	0.72
1:I:135:LEU:HD11	3:I:300:HOH:O	1.89	0.72
1:D:216:HIS:O	1:D:219:LYS:HE2	1.90	0.72
1:E:177:LEU:HD23	1:E:180:ARG:NH2	2.05	0.72
1:B:64:GLY:HA3	1:B:71:LEU:HD22	1.74	0.70
1:I:86:LEU:O	1:I:135:LEU:HD22	1.92	0.70
1:C:4:SER:N	3:C:743:HOH:O	2.25	0.70
1:D:202:PRO:O	1:D:202:PRO:HG2	1.90	0.70
1:F:30:ARG:NH2	1:F:55:GLY:HA3	2.06	0.70
1:B:180:ARG:NH1	1:B:180:ARG:HG3	1.99	0.70
1:A:38:THR:HG21	1:A:75:LEU:HD11	1.73	0.69
1:F:91:ASN:HD21	1:F:128:GLN:HE22	1.40	0.69
1:B:40:ARG:HB2	2:B:601:NAP:O2X	1.92	0.69
1:I:86:LEU:O	1:I:135:LEU:CD2	2.42	0.68
1:A:81:ARG:HD2	3:A:800:HOH:O	1.95	0.67
1:D:91:ASN:HD21	1:D:128:GLN:HE22	1.41	0.66
1:D:44:ALA:O	1:D:47:GLU:HG3	1.97	0.65
1:G:198:PHE:CA	1:G:201:LEU:HD13	2.17	0.65
1:D:38:THR:HG21	1:D:75:LEU:HD11	1.78	0.65
1:C:110:TRP:CZ2	1:C:114:LEU:HD11	2.31	0.65
1:E:177:LEU:HD23	1:E:180:ARG:HH21	1.61	0.65
1:D:152:GLY:N	1:E:255:VAL:HG13	2.12	0.65
1:B:91:ASN:HD21	1:B:128:GLN:HE22	1.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASN:HD21	1:C:128:GLN:HE22	1.44	0.64
1:B:30:ARG:NH1	1:B:30:ARG:HG2	2.10	0.64
1:I:49:THR:HG21	1:I:61:ALA:HB2	1.80	0.64
1:D:202:PRO:O	1:D:202:PRO:HD2	1.97	0.63
1:F:135:LEU:CD1	1:F:135:LEU:O	2.46	0.63
1:I:99:MET:HE1	1:I:156:VAL:CG1	2.28	0.63
1:F:35:VAL:HG12	1:F:37:VAL:HG13	1.81	0.63
1:E:177:LEU:CD2	1:E:180:ARG:HH21	2.11	0.63
1:E:34:LYS:HE3	1:E:58:GLU:OE2	1.99	0.62
1:C:110:TRP:NE1	1:C:114:LEU:HD12	2.15	0.62
1:G:197:ASN:O	1:G:201:LEU:HD12	1.99	0.62
1:E:205:ALA:HB1	1:E:206:PRO:HD2	1.81	0.62
1:F:34:LYS:HE3	1:F:58:GLU:OE2	2.00	0.62
1:A:82:ARG:NH2	3:A:336:HOH:O	2.31	0.62
1:A:135:LEU:CD2	1:A:135:LEU:N	2.63	0.61
1:G:199:ALA:HA	1:G:208:THR:HG21	1.83	0.61
1:I:54:GLY:H	1:I:56:GLY:H	1.48	0.60
1:A:201:LEU:HB3	1:A:202:PRO:HD2	1.84	0.60
1:A:81:ARG:NH2	1:D:193:ASP:OD1	2.34	0.60
1:B:77:GLU:O	1:B:81:ARG:HG3	2.01	0.59
1:B:135:LEU:HD23	1:B:135:LEU:N	2.16	0.59
1:A:81:ARG:HH22	1:D:193:ASP:CG	2.05	0.59
1:F:26:LEU:HD23	1:F:52:ILE:HD13	1.85	0.59
1:F:247:LEU:HD23	1:F:247:LEU:C	2.21	0.59
1:I:134:ALA:C	1:I:135:LEU:HD12	2.22	0.59
1:A:257:LYS:CD	3:B:742:HOH:O	2.50	0.59
1:A:110:TRP:NE1	1:A:114:LEU:HD12	2.18	0.58
1:E:96:LEU:HB3	1:E:99:MET:HE3	1.84	0.58
1:C:4:SER:N	3:C:304:HOH:O	2.35	0.58
1:E:38:THR:HG21	1:E:75:LEU:HD11	1.84	0.58
1:D:110:TRP:NE1	1:D:114:LEU:HD12	2.18	0.58
1:G:5:ARG:HD2	1:G:31:GLU:OE1	2.02	0.58
1:F:96:LEU:CB	1:F:99:MET:HE3	2.20	0.58
1:G:30:ARG:NH2	1:G:55:GLY:HA3	2.19	0.57
1:C:54:GLY:N	1:C:56:GLY:H	2.02	0.57
1:A:135:LEU:N	1:A:135:LEU:HD22	2.20	0.56
1:C:48:LEU:O	1:C:52:ILE:HG13	2.05	0.56
1:C:110:TRP:CE2	1:C:114:LEU:HD11	2.40	0.56
1:F:135:LEU:C	1:F:135:LEU:HD12	2.26	0.56
1:A:5:ARG:NH2	1:A:229:GLU:OE1	2.35	0.56
1:I:201:LEU:HB3	1:I:202:PRO:HD2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:471:HOH:O	1:E:257:LYS:CD	2.53	0.55
1:B:26:LEU:O	1:B:30:ARG:HG2	2.06	0.55
1:F:40:ARG:HB2	2:F:601:NAP:O2X	2.06	0.55
1:A:5:ARG:HD3	1:A:31:GLU:OE1	2.07	0.55
1:A:50:ASP:O	1:A:53:ALA:O	2.25	0.54
1:I:99:MET:HE2	1:I:156:VAL:HG12	1.87	0.54
1:C:152:GLY:N	1:G:255:VAL:HG13	2.22	0.54
1:G:199:ALA:HA	1:G:208:THR:CG2	2.37	0.54
1:E:9:LYS:HA	1:E:87:ASP:OD2	2.08	0.54
1:E:30:ARG:NH2	1:E:55:GLY:HA3	2.22	0.54
1:C:34:LYS:HE3	1:C:58:GLU:OE2	2.09	0.53
1:G:34:LYS:HE3	1:G:58:GLU:OE2	2.09	0.53
1:G:255:VAL:CG1	1:G:255:VAL:O	2.56	0.53
1:C:110:TRP:NE1	1:C:114:LEU:CD1	2.72	0.52
1:G:5:ARG:HD2	1:G:31:GLU:CD	2.30	0.52
1:G:35:VAL:HG12	1:G:37:VAL:HG13	1.90	0.52
1:B:26:LEU:CD1	1:B:30:ARG:NH2	2.72	0.52
1:E:194:THR:HB	1:E:195:PRO:HD2	1.92	0.52
1:E:40:ARG:HB2	2:E:601:NAP:O2X	2.10	0.52
1:G:255:VAL:HG12	1:G:255:VAL:O	2.09	0.52
1:C:216:HIS:O	1:C:219:LYS:HE2	2.09	0.52
1:G:14:THR:HG22	1:G:38:THR:CG2	2.39	0.51
1:I:111:ARG:HD3	3:I:848:HOH:O	2.09	0.51
1:C:110:TRP:CE2	1:C:114:LEU:CD1	2.94	0.51
1:G:213:GLU:HG2	1:G:220:ARG:HA	1.92	0.51
1:B:185:ASN:HD22	1:B:245:ALA:H	1.59	0.51
1:C:34:LYS:HG2	3:C:578:HOH:O	2.11	0.51
1:F:77:GLU:O	1:F:81:ARG:HG2	2.11	0.51
1:G:36:VAL:HG21	1:G:79:ALA:HB2	1.93	0.50
1:I:38:THR:HG21	1:I:75:LEU:HD11	1.92	0.50
1:A:54:GLY:H	1:A:56:GLY:H	1.59	0.50
1:F:64:GLY:HA3	1:F:71:LEU:HD22	1.92	0.50
1:A:187:LEU:CD1	1:A:247:LEU:HD22	2.41	0.50
1:A:82:ARG:HH11	1:A:82:ARG:HG3	1.76	0.50
1:B:209:ARG:NH1	3:B:370:HOH:O	2.44	0.50
1:B:34:LYS:HE3	1:B:58:GLU:OE2	2.12	0.50
1:F:135:LEU:O	1:F:135:LEU:HD12	2.10	0.50
1:F:96:LEU:HB3	1:F:99:MET:CE	2.23	0.50
1:D:171:GLN:HB3	1:F:255:VAL:HG11	1.94	0.50
1:C:66:VAL:HB	2:C:601:NAP:C2A	2.43	0.49
1:F:30:ARG:NH2	1:F:55:GLY:CA	2.74	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:VAL:O	1:F:255:VAL:HG12	2.11	0.49
1:I:131:ALA:O	1:I:135:LEU:HD13	2.12	0.49
1:A:38:THR:HB	1:A:75:LEU:HD21	1.95	0.49
1:E:197:ASN:OD1	1:E:199:ALA:HB3	2.13	0.48
1:F:137:GLY:HA3	1:F:138:GLY:HA2	1.71	0.48
1:A:37:VAL:HG23	1:A:45:LEU:HD22	1.94	0.48
1:I:5:ARG:HD3	1:I:31:GLU:OE1	2.14	0.48
1:B:26:LEU:HD11	1:B:30:ARG:NH2	2.28	0.48
1:D:152:GLY:H	1:E:255:VAL:HG13	1.78	0.48
1:E:195:PRO:HD2	2:E:601:NAP:O2A	2.14	0.47
1:G:66:VAL:HB	2:G:601:NAP:C2A	2.44	0.47
1:G:4:SER:HB2	1:G:7:GLU:HB2	1.96	0.47
1:I:194:THR:HB	1:I:195:PRO:HD2	1.97	0.47
1:A:110:TRP:NE1	1:A:114:LEU:CD1	2.78	0.47
1:F:26:LEU:CD2	1:F:52:ILE:HD13	2.44	0.47
1:B:17:SER:HB3	1:B:39:ALA:CB	2.45	0.47
1:E:34:LYS:CE	1:E:58:GLU:OE2	2.63	0.47
1:E:111:ARG:NH2	3:E:785:HOH:O	2.33	0.47
2:E:601:NAP:O1N	2:E:601:NAP:H2N	2.14	0.47
1:G:135:LEU:HD12	1:G:135:LEU:N	2.29	0.47
1:G:9:LYS:HA	1:G:87:ASP:OD2	2.14	0.47
1:F:197:ASN:OD1	1:F:199:ALA:HB3	2.15	0.47
1:E:53:ALA:C	1:E:55:GLY:H	2.18	0.46
1:F:135:LEU:O	1:F:135:LEU:HD13	2.13	0.46
1:A:112:GLU:HG3	3:A:293:HOH:O	2.15	0.46
1:G:40:ARG:HB2	2:G:601:NAP:O2X	2.15	0.46
1:F:255:VAL:CG1	1:I:152:GLY:N	2.78	0.46
1:F:255:VAL:HG13	1:I:152:GLY:N	2.30	0.46
1:I:38:THR:HB	1:I:75:LEU:HD21	1.97	0.46
1:F:185:ASN:HD22	1:F:245:ALA:H	1.64	0.46
1:I:185:ASN:HD22	1:I:245:ALA:H	1.64	0.46
1:E:35:VAL:HG12	1:E:37:VAL:HG13	1.97	0.46
1:G:38:THR:HG21	1:G:75:LEU:HD11	1.98	0.46
1:I:64:GLY:C	1:I:71:LEU:HD22	2.36	0.46
1:A:64:GLY:HA3	1:A:71:LEU:HD13	1.98	0.46
1:D:185:ASN:HD22	1:D:245:ALA:H	1.65	0.45
1:C:36:VAL:HG12	1:C:75:LEU:HD22	1.98	0.45
1:D:257:LYS:CD	3:E:604:HOH:O	2.64	0.45
1:E:29:ALA:CB	1:E:52:ILE:HD13	2.46	0.45
1:C:257:LYS:CD	3:G:546:HOH:O	2.65	0.45
1:D:177:LEU:HD23	1:D:180:ARG:HH21	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:114:LEU:HD23	1:G:162:SER:CB	2.47	0.45
1:E:255:VAL:O	1:E:255:VAL:HG12	2.17	0.44
1:E:201:LEU:HB3	1:E:202:PRO:HD2	2.00	0.44
1:G:197:ASN:HD21	1:G:212:VAL:HG11	1.81	0.44
1:F:58:GLU:OE1	1:F:82:ARG:NH2	2.47	0.44
1:G:77:GLU:O	1:G:81:ARG:HG2	2.17	0.44
1:I:202:PRO:O	1:I:202:PRO:HG2	2.17	0.44
1:A:185:ASN:ND2	1:A:245:ALA:H	2.16	0.44
1:B:14:THR:HG22	1:B:38:THR:CG2	2.48	0.44
1:B:255:VAL:O	1:B:255:VAL:HG12	2.17	0.44
1:D:255:VAL:CG1	1:D:255:VAL:O	2.65	0.44
1:D:64:GLY:HA3	1:D:71:LEU:HD22	1.99	0.44
2:F:601:NAP:H2A	3:F:309:HOH:O	2.17	0.44
1:D:190:GLY:H	1:D:250:ASP:HA	1.83	0.44
1:A:185:ASN:HD22	1:A:245:ALA:H	1.64	0.44
1:I:45:LEU:O	1:I:49:THR:HG23	2.18	0.44
1:E:34:LYS:HD2	1:E:83:PHE:CE1	2.53	0.43
1:F:73:GLU:O	1:F:77:GLU:HG2	2.17	0.43
1:I:36:VAL:HG21	1:I:79:ALA:HB2	2.00	0.43
1:G:96:LEU:HD13	1:G:99:MET:HE3	2.00	0.43
1:D:36:VAL:HG12	1:D:75:LEU:HD22	2.01	0.43
1:B:35:VAL:HG12	1:B:37:VAL:HG13	2.00	0.43
1:E:66:VAL:HB	2:E:601:NAP:C2A	2.48	0.43
1:C:85:GLY:HA3	1:C:135:LEU:HD11	2.01	0.43
1:E:30:ARG:HG2	3:E:711:HOH:O	2.18	0.43
1:C:152:GLY:H	1:G:255:VAL:HG13	1.84	0.43
1:B:213:GLU:HG2	1:B:221:ILE:HG13	2.01	0.43
1:G:96:LEU:HB3	1:G:99:MET:CE	2.24	0.43
1:I:134:ALA:HB3	1:I:135:LEU:CD1	2.48	0.43
1:E:153:PHE:O	1:E:156:VAL:HG22	2.19	0.43
1:F:135:LEU:CD1	1:F:135:LEU:C	2.86	0.43
1:C:38:THR:HG21	1:C:75:LEU:HD11	2.00	0.43
1:E:185:ASN:HD22	1:E:245:ALA:H	1.66	0.43
3:F:322:HOH:O	1:I:257:LYS:CD	2.66	0.43
1:A:107:VAL:O	1:A:111:ARG:HG3	2.19	0.42
1:B:4:SER:HB2	1:B:7:GLU:HB2	2.01	0.42
1:E:255:VAL:CG1	1:E:255:VAL:O	2.67	0.42
1:F:30:ARG:HD3	1:F:30:ARG:HA	1.38	0.42
1:A:135:LEU:CD2	1:A:135:LEU:H	2.32	0.42
1:I:96:LEU:HD22	1:I:99:MET:HE3	2.01	0.42
1:C:194:THR:HB	1:C:195:PRO:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:VAL:HB	2:D:601:NAP:C2A	2.50	0.42
1:E:205:ALA:HB1	1:E:206:PRO:CD	2.49	0.42
1:E:191:GLY:C	1:E:221:ILE:HG23	2.39	0.42
1:E:17:SER:HB3	1:E:39:ALA:CB	2.49	0.42
1:D:38:THR:CG2	1:D:75:LEU:HD11	2.49	0.42
1:D:152:GLY:H	1:E:255:VAL:CG1	2.32	0.42
1:E:52:ILE:HG21	1:E:59:ALA:HB2	2.00	0.42
1:D:152:GLY:N	1:E:255:VAL:CG1	2.81	0.42
1:E:80:VAL:HG22	1:E:85:GLY:HA2	2.01	0.42
1:E:99:MET:HE1	1:E:156:VAL:HG12	1.96	0.42
1:B:185:ASN:ND2	1:B:245:ALA:H	2.18	0.42
1:D:247:LEU:HD23	1:D:247:LEU:C	2.40	0.42
1:F:257:LYS:CD	3:I:430:HOH:O	2.67	0.42
1:G:30:ARG:HD2	1:G:30:ARG:HA	1.67	0.42
1:I:131:ALA:O	1:I:135:LEU:CD1	2.67	0.42
1:F:185:ASN:HD21	1:F:243:THR:HA	1.85	0.41
1:B:153:PHE:O	1:B:156:VAL:HG22	2.20	0.41
1:E:29:ALA:HB3	1:E:52:ILE:HD13	2.02	0.41
1:E:38:THR:HB	1:E:75:LEU:HD21	2.01	0.41
1:I:209:ARG:O	1:I:213:GLU:HG2	2.20	0.41
1:A:64:GLY:C	1:A:71:LEU:HD22	2.40	0.41
1:B:135:LEU:CD2	1:B:135:LEU:N	2.83	0.41
1:E:118:LEU:HD23	1:F:114:LEU:HD11	2.01	0.41
1:F:197:ASN:HD21	1:F:212:VAL:HG11	1.86	0.41
1:F:30:ARG:CZ	1:F:55:GLY:HA3	2.50	0.41
1:A:187:LEU:HD12	1:A:247:LEU:HD22	2.01	0.41
1:F:247:LEU:C	1:F:247:LEU:CD2	2.88	0.41
1:I:185:ASN:HD21	1:I:243:THR:HA	1.86	0.41
1:D:202:PRO:HA	1:D:203:GLY:HA2	1.86	0.41
1:I:5:ARG:NH2	1:I:229:GLU:OE1	2.46	0.41
1:B:64:GLY:CA	1:B:71:LEU:HD22	2.47	0.41
1:C:54:GLY:CA	1:C:56:GLY:H	2.34	0.40
1:D:255:VAL:HG12	1:F:175:VAL:HG23	2.02	0.40
1:G:66:VAL:HG12	2:G:601:NAP:N1A	2.36	0.40
1:E:38:THR:CG2	1:E:75:LEU:HD11	2.51	0.40
1:I:185:ASN:ND2	1:I:245:ALA:H	2.19	0.40
1:B:66:VAL:HG11	1:B:93:ALA:HB1	2.03	0.40
1:C:40:ARG:HB2	2:C:601:NAP:O2X	2.22	0.40
1:D:185:ASN:HD21	1:D:243:THR:HA	1.87	0.40
1:D:110:TRP:CZ2	1:D:114:LEU:HD11	2.57	0.40

There are no symmetry-related clashes.

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	252/280 (90%)	246 (98%)	6 (2%)	0	100	100
1	B	244/280 (87%)	238 (98%)	5 (2%)	1 (0%)	38	25
1	C	252/280 (90%)	248 (98%)	4 (2%)	0	100	100
1	D	252/280 (90%)	245 (97%)	7 (3%)	0	100	100
1	E	252/280 (90%)	248 (98%)	4 (2%)	0	100	100
1	F	250/280 (89%)	245 (98%)	5 (2%)	0	100	100
1	G	247/280 (88%)	242 (98%)	5 (2%)	0	100	100
1	I	252/280 (90%)	246 (98%)	6 (2%)	0	100	100
All	All	2001/2240 (89%)	1958 (98%)	42 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	GLY

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	163/188 (87%)	160 (98%)	3 (2%)	64	55
1	B	158/188 (84%)	154 (98%)	4 (2%)	53	41
1	C	163/188 (87%)	161 (99%)	2 (1%)	75	71
1	D	163/188 (87%)	161 (99%)	2 (1%)	75	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	162/188 (86%)	157 (97%)	5 (3%)	45	31
1	F	160/188 (85%)	158 (99%)	2 (1%)	73	68
1	G	160/188 (85%)	156 (98%)	4 (2%)	53	41
1	I	163/188 (87%)	157 (96%)	6 (4%)	39	24
All	All	1292/1504 (86%)	1264 (98%)	28 (2%)	57	47

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

Mol	Chain	Res	Type
1	A	47	GLU
1	A	82	ARG
1	A	135	LEU
1	B	30	ARG
1	B	75	LEU
1	B	135	LEU
1	B	180	ARG
1	C	47	GLU
1	C	66	VAL
1	D	47	GLU
1	D	202	PRO
1	E	26	LEU
1	E	47	GLU
1	E	52	ILE
1	E	114	LEU
1	E	135	LEU
1	F	75	LEU
1	F	82	ARG
1	G	26	LEU
1	G	30	ARG
1	G	51	GLU
1	G	75	LEU
1	I	47	GLU
1	I	52	ILE
1	I	112	GLU
1	I	135	LEU
1	I	202	PRO
1	I	213	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	185	ASN
1	B	91	ASN
1	B	185	ASN
1	C	91	ASN
1	C	185	ASN
1	D	91	ASN
1	D	185	ASN
1	E	91	ASN
1	E	185	ASN
1	F	91	ASN
1	F	185	ASN
1	G	91	ASN
1	G	185	ASN
1	I	43	ASN
1	I	91	ASN
1	I	185	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
2	NAP	A	601	-	44,52,52	2.57	10 (22%)	51,80,80	2.99	5 (9%)
2	NAP	B	601	-	44,52,52	2.69	11 (25%)	51,80,80	2.84	7 (13%)
2	NAP	C	601	-	44,52,52	2.77	9 (20%)	51,80,80	2.62	4 (7%)
2	NAP	D	601	-	44,52,52	2.37	9 (20%)	51,80,80	2.82	5 (9%)
2	NAP	E	601	-	44,52,52	2.62	9 (20%)	51,80,80	2.92	7 (13%)
2	NAP	F	601	-	44,52,52	2.66	9 (20%)	51,80,80	3.10	5 (9%)
2	NAP	G	601	-	44,52,52	2.61	9 (20%)	51,80,80	2.87	6 (11%)
2	NAP	I	601	-	44,52,52	2.80	14 (31%)	51,80,80	2.99	9 (17%)

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	601	-	-	0/27/67/67	0/5/5/5
2	NAP	B	601	-	-	0/27/67/67	0/5/5/5
2	NAP	C	601	-	-	0/27/67/67	0/5/5/5
2	NAP	D	601	-	-	0/27/67/67	0/5/5/5
2	NAP	E	601	-	-	0/27/67/67	0/5/5/5
2	NAP	F	601	-	-	0/27/67/67	0/5/5/5
2	NAP	G	601	-	-	0/27/67/67	0/5/5/5
2	NAP	I	601	-	-	0/27/67/67	0/5/5/5

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	NAP	C3N-C7N	-4.65	1.43	1.50
2	C	601	NAP	C3N-C7N	-4.45	1.43	1.50
2	A	601	NAP	C3N-C7N	-4.21	1.44	1.50
2	B	601	NAP	C3N-C7N	-4.05	1.44	1.50
2	G	601	NAP	C3N-C7N	-4.00	1.44	1.50
2	D	601	NAP	C3N-C7N	-3.61	1.44	1.50
2	I	601	NAP	C3N-C7N	-3.29	1.45	1.50
2	E	601	NAP	C3N-C7N	-3.02	1.45	1.50
2	F	601	NAP	C5A-C4A	-2.29	1.35	1.40
2	I	601	NAP	P2B-O2X	-2.24	1.45	1.54
2	G	601	NAP	O4B-C4B	-2.23	1.40	1.45
2	C	601	NAP	C2D-C1D	-2.12	1.50	1.53
2	I	601	NAP	C5A-C4A	-2.12	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	NAP	P2B-O2X	-2.09	1.46	1.54
2	I	601	NAP	C3B-C4B	-2.04	1.47	1.53
2	D	601	NAP	C5A-C4A	-2.02	1.36	1.40
2	A	601	NAP	O4B-C1B	2.02	1.44	1.41
2	E	601	NAP	PA-O5B	2.03	1.67	1.59
2	F	601	NAP	C5N-C4N	2.04	1.42	1.38
2	A	601	NAP	C6N-C5N	2.07	1.43	1.38
2	F	601	NAP	C4N-C3N	2.07	1.42	1.39
2	B	601	NAP	PA-O5B	2.08	1.68	1.59
2	C	601	NAP	C6N-C5N	2.11	1.43	1.38
2	D	601	NAP	C6N-N1N	2.12	1.40	1.35
2	G	601	NAP	PN-O5D	2.13	1.68	1.59
2	F	601	NAP	PN-O5D	2.14	1.68	1.59
2	B	601	NAP	PN-O5D	2.15	1.68	1.59
2	B	601	NAP	C4N-C3N	2.16	1.42	1.39
2	I	601	NAP	C5N-C4N	2.22	1.43	1.38
2	G	601	NAP	C4N-C3N	2.25	1.43	1.39
2	A	601	NAP	PN-O5D	2.25	1.68	1.59
2	C	601	NAP	O4B-C1B	2.31	1.44	1.41
2	G	601	NAP	P2B-O2B	2.37	1.63	1.59
2	I	601	NAP	PN-O5D	2.40	1.69	1.59
2	D	601	NAP	PN-O5D	2.42	1.69	1.59
2	E	601	NAP	PN-O5D	2.45	1.69	1.59
2	E	601	NAP	C4N-C3N	2.46	1.43	1.39
2	A	601	NAP	C3D-C4D	2.50	1.59	1.53
2	A	601	NAP	O3B-C3B	2.52	1.48	1.43
2	I	601	NAP	C2D-C3D	2.58	1.60	1.53
2	A	601	NAP	C6N-N1N	2.59	1.42	1.35
2	I	601	NAP	C6N-C5N	2.66	1.44	1.38
2	B	601	NAP	O3D-C3D	2.71	1.49	1.43
2	D	601	NAP	O3D-C3D	2.77	1.49	1.43
2	I	601	NAP	O3B-C3B	2.80	1.49	1.43
2	B	601	NAP	O4B-C1B	2.80	1.45	1.41
2	I	601	NAP	O4B-C1B	2.90	1.45	1.41
2	C	601	NAP	O4D-C1D	2.95	1.45	1.41
2	I	601	NAP	P2B-O2B	2.96	1.64	1.59
2	G	601	NAP	C6N-N1N	3.03	1.43	1.35
2	B	601	NAP	O4D-C1D	3.06	1.45	1.41
2	E	601	NAP	O4D-C1D	3.47	1.46	1.41
2	F	601	NAP	P2B-O2B	3.53	1.65	1.59
2	B	601	NAP	P2B-O2B	3.60	1.65	1.59
2	I	601	NAP	C6N-N1N	3.61	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	NAP	C6N-N1N	3.65	1.44	1.35
2	E	601	NAP	P2B-O2B	3.69	1.66	1.59
2	B	601	NAP	C6N-N1N	3.75	1.45	1.35
2	D	601	NAP	O3B-C3B	3.76	1.51	1.43
2	F	601	NAP	C6N-N1N	3.80	1.45	1.35
2	C	601	NAP	P2B-O2B	4.69	1.67	1.59
2	A	601	NAP	P2B-O2B	4.88	1.68	1.59
2	G	601	NAP	O4B-C1B	5.25	1.48	1.41
2	C	601	NAP	O3B-C3B	6.45	1.57	1.43
2	D	601	NAP	C2A-N3A	8.56	1.46	1.32
2	G	601	NAP	C2A-N1A	8.77	1.50	1.33
2	F	601	NAP	C2A-N1A	8.83	1.50	1.33
2	B	601	NAP	C2A-N1A	8.83	1.50	1.33
2	A	601	NAP	C2A-N1A	8.91	1.50	1.33
2	D	601	NAP	C2A-N1A	9.22	1.51	1.33
2	C	601	NAP	C2A-N1A	9.38	1.51	1.33
2	C	601	NAP	C2A-N3A	9.59	1.48	1.32
2	E	601	NAP	C2A-N1A	9.82	1.52	1.33
2	A	601	NAP	C2A-N3A	10.08	1.48	1.32
2	I	601	NAP	C2A-N1A	10.18	1.53	1.33
2	E	601	NAP	C2A-N3A	10.33	1.49	1.32
2	G	601	NAP	C2A-N3A	10.42	1.49	1.32
2	F	601	NAP	C2A-N3A	11.06	1.50	1.32
2	I	601	NAP	C2A-N3A	11.11	1.50	1.32
2	B	601	NAP	C2A-N3A	11.16	1.50	1.32

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	NAP	N3A-C2A-N1A	-19.89	111.54	128.86
2	A	601	NAP	N3A-C2A-N1A	-19.41	111.95	128.86
2	I	601	NAP	N3A-C2A-N1A	-19.13	112.20	128.86
2	D	601	NAP	N3A-C2A-N1A	-18.16	113.05	128.86
2	E	601	NAP	N3A-C2A-N1A	-17.95	113.22	128.86
2	G	601	NAP	N3A-C2A-N1A	-17.91	113.26	128.86
2	B	601	NAP	N3A-C2A-N1A	-17.68	113.47	128.86
2	C	601	NAP	N3A-C2A-N1A	-17.06	114.00	128.86
2	E	601	NAP	C1B-N9A-C4A	-5.62	116.92	126.64
2	B	601	NAP	C1B-N9A-C4A	-5.03	117.94	126.64
2	F	601	NAP	C1B-N9A-C4A	-4.47	118.92	126.64
2	D	601	NAP	C1B-N9A-C4A	-3.82	120.04	126.64
2	G	601	NAP	C4A-C5A-N7A	-3.46	106.06	109.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAP	C4D-O4D-C1D	-3.28	106.28	109.77
2	I	601	NAP	O7N-C7N-N7N	-3.13	118.13	122.58
2	C	601	NAP	C4A-C5A-N7A	-3.11	106.41	109.41
2	F	601	NAP	C3N-C7N-N7N	-2.99	114.36	117.77
2	F	601	NAP	C4A-C5A-N7A	-2.83	106.67	109.41
2	G	601	NAP	C4D-O4D-C1D	-2.55	107.06	109.77
2	A	601	NAP	C1B-N9A-C4A	-2.48	122.36	126.64
2	I	601	NAP	C4A-C5A-N7A	-2.43	107.07	109.41
2	I	601	NAP	C4D-O4D-C1D	-2.35	107.27	109.77
2	E	601	NAP	O2X-P2B-O2B	-2.33	95.41	106.00
2	C	601	NAP	C4D-O4D-C1D	-2.25	107.37	109.77
2	A	601	NAP	C4D-O4D-C1D	-2.25	107.38	109.77
2	E	601	NAP	C4A-C5A-N7A	-2.25	107.24	109.41
2	I	601	NAP	C1B-N9A-C4A	-2.25	122.75	126.64
2	D	601	NAP	C4D-O4D-C1D	-2.24	107.38	109.77
2	G	601	NAP	C1B-N9A-C4A	-2.24	122.77	126.64
2	B	601	NAP	O3B-C3B-C2B	-2.18	104.99	111.18
2	C	601	NAP	C1B-N9A-C4A	-2.16	122.91	126.64
2	I	601	NAP	O4B-C1B-C2B	-2.12	102.89	106.59
2	B	601	NAP	C4A-C5A-N7A	-2.09	107.39	109.41
2	D	601	NAP	C5B-C4B-C3B	-2.04	107.52	115.29
2	A	601	NAP	O3X-P2B-O2X	2.04	115.83	107.61
2	I	601	NAP	C5N-C4N-C3N	2.11	122.83	120.35
2	E	601	NAP	O3X-P2B-O2X	2.17	116.35	107.61
2	I	601	NAP	O2X-P2B-O1X	2.24	119.25	110.50
2	G	601	NAP	O7N-C7N-C3N	2.32	122.33	119.62
2	B	601	NAP	C5N-C4N-C3N	2.52	123.31	120.35
2	A	601	NAP	C5N-C4N-C3N	2.72	123.55	120.35
2	I	601	NAP	C3N-C7N-N7N	2.73	120.90	117.77
2	D	601	NAP	O7N-C7N-C3N	2.84	122.94	119.62
2	E	601	NAP	O7N-C7N-C3N	3.00	123.13	119.62
2	B	601	NAP	O7N-C7N-C3N	3.04	123.17	119.62
2	E	601	NAP	C5N-C4N-C3N	3.20	124.11	120.35
2	G	601	NAP	C5N-C4N-C3N	3.26	124.18	120.35
2	F	601	NAP	O7N-C7N-C3N	3.55	123.78	119.62

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
2	B	601	NAP	1	0
2	C	601	NAP	2	0
2	D	601	NAP	1	0
2	E	601	NAP	4	0
2	F	601	NAP	2	0
2	G	601	NAP	3	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	254/280 (90%)	0.09	11 (4%)	36	45	13, 21, 33, 41	0
1	B	248/280 (88%)	0.30	19 (7%)	14	20	15, 25, 43, 56	0
1	C	254/280 (90%)	0.10	10 (3%)	40	49	12, 20, 31, 40	0
1	D	254/280 (90%)	0.12	11 (4%)	36	45	12, 21, 33, 45	0
1	E	254/280 (90%)	0.48	22 (8%)	11	16	15, 25, 50, 70	0
1	F	254/280 (90%)	0.35	22 (8%)	11	16	15, 24, 43, 60	0
1	G	251/280 (89%)	0.38	22 (8%)	11	16	15, 24, 43, 63	0
1	I	254/280 (90%)	0.10	10 (3%)	40	49	12, 21, 33, 42	0
All	All	2023/2240 (90%)	0.24	127 (6%)	21	28	12, 23, 40, 70	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	204	ALA	7.5
1	E	202	PRO	7.0
1	E	205	ALA	6.2
1	G	201	LEU	6.0
1	E	203	GLY	5.8
1	E	196	ALA	5.7
1	G	205	ALA	5.7
1	G	198	PHE	5.0
1	F	199	ALA	4.8
1	E	201	LEU	4.8
1	B	195	PRO	4.8
1	E	208	THR	4.5
1	E	206	PRO	4.5
1	G	206	PRO	4.5
1	E	198	PHE	4.5
1	G	195	PRO	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	202	PRO	4.3
1	F	206	PRO	4.3
1	G	194	THR	4.2
1	G	199	ALA	4.2
1	A	203	GLY	4.1
1	F	208	THR	4.1
1	G	196	ALA	4.0
1	F	259	ALA	3.9
1	G	200	ASN	3.8
1	B	135	LEU	3.8
1	E	209	ARG	3.8
1	I	53	ALA	3.8
1	E	195	PRO	3.6
1	C	246	ALA	3.6
1	E	80	VAL	3.6
1	E	54	GLY	3.6
1	B	200	ASN	3.5
1	F	198	PHE	3.5
1	G	208	THR	3.5
1	B	134	ALA	3.5
1	E	135	LEU	3.4
1	B	54	GLY	3.4
1	G	135	LEU	3.4
1	G	207	GLU	3.3
1	F	195	PRO	3.2
1	E	199	ALA	3.2
1	G	211	PHE	3.2
1	B	208	THR	3.1
1	G	209	ARG	3.1
1	F	209	ARG	3.1
1	F	200	ASN	3.1
1	F	211	PHE	3.1
1	A	188	LEU	2.9
1	B	209	ARG	2.9
1	C	248	LEU	2.9
1	D	247	LEU	2.9
1	C	203	GLY	2.9
1	G	246	ALA	2.8
1	B	199	ALA	2.8
1	C	245	ALA	2.8
1	F	135	LEU	2.8
1	G	18	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	196	ALA	2.7
1	B	247	LEU	2.7
1	E	30	ARG	2.7
1	E	207	GLU	2.7
1	D	201	LEU	2.7
1	E	211	PHE	2.7
1	B	57	GLY	2.6
1	I	202	PRO	2.6
1	A	167	ILE	2.5
1	A	248	LEU	2.5
1	C	188	LEU	2.5
1	B	81	ARG	2.5
1	E	47	GLU	2.5
1	B	255	VAL	2.4
1	D	248	LEU	2.4
1	I	135	LEU	2.4
1	F	210	GLY	2.4
1	G	245	ALA	2.4
1	F	81	ARG	2.4
1	F	194	THR	2.4
1	D	188	LEU	2.4
1	A	202	PRO	2.4
1	E	81	ARG	2.4
1	G	85	GLY	2.4
1	D	202	PRO	2.4
1	C	149	HIS	2.4
1	B	167	ILE	2.4
1	B	211	PHE	2.3
1	G	197	ASN	2.3
1	F	246	ALA	2.3
1	E	200	ASN	2.3
1	I	201	LEU	2.3
1	B	30	ARG	2.3
1	I	248	LEU	2.3
1	B	55	GLY	2.3
1	D	150	THR	2.2
1	I	164	ALA	2.2
1	D	203	GLY	2.2
1	F	261	ASN	2.2
1	F	30	ARG	2.2
1	E	18	SER	2.2
1	D	246	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	248	LEU	2.2
1	I	188	LEU	2.2
1	I	149	HIS	2.2
1	F	196	ALA	2.2
1	A	43	ASN	2.2
1	F	197	ASN	2.2
1	B	194	THR	2.2
1	A	149	HIS	2.1
1	C	167	ILE	2.1
1	I	167	ILE	2.1
1	A	135	LEU	2.1
1	B	246	ALA	2.1
1	C	164	ALA	2.1
1	D	164	ALA	2.1
1	G	149	HIS	2.1
1	A	53	ALA	2.1
1	C	247	LEU	2.1
1	I	246	ALA	2.1
1	F	80	VAL	2.1
1	A	247	LEU	2.1
1	G	248	LEU	2.1
1	F	54	GLY	2.1
1	G	247	LEU	2.1
1	F	207	GLU	2.0
1	A	246	ALA	2.0
1	D	167	ILE	2.0
1	D	149	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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
2	NAP	F	601	48/48	0.91	0.19	1.32	29,41,46,51	0
2	NAP	E	601	48/48	0.85	0.21	1.25	30,37,49,52	0
2	NAP	G	601	48/48	0.88	0.21	1.05	28,39,45,46	0
2	NAP	B	601	48/48	0.90	0.19	0.92	30,39,47,48	0
2	NAP	I	601	48/48	0.94	0.10	-0.10	16,24,30,33	0
2	NAP	D	601	48/48	0.96	0.08	-0.64	15,23,30,35	0
2	NAP	A	601	48/48	0.96	0.09	-0.68	19,25,32,35	0
2	NAP	C	601	48/48	0.96	0.09	-0.79	18,23,31,34	0

6.5 Other polymers ⓘ

There are no such residues in this entry.