



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 04:07 am BST

PDB ID : 3HZN
Title : Structure of the Salmonella typhimurium nfnB dihydropteridine reductase
Authors : Anderson, S.M.; Wawrzak, Z.; Onopriyenko, O.; Skarina, T.; Anderson, W.F.; Savchenko, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2009-06-23
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

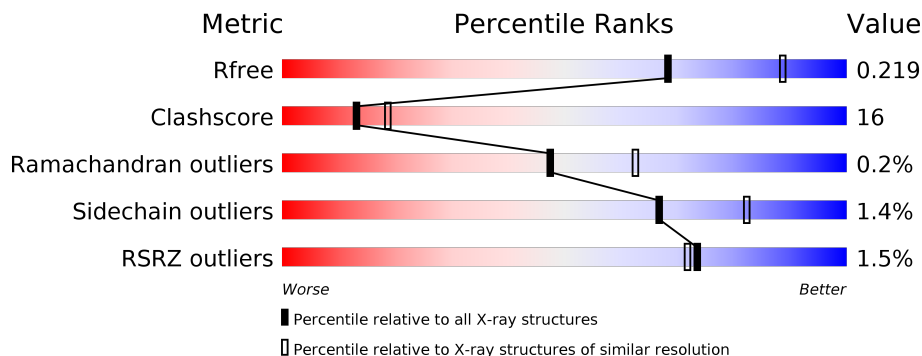
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 respectively. 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	220	
1	B	220	
1	C	220	
1	D	220	
1	E	220	
1	F	220	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	220	
1	H	220	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TLA	H	218	-	-	X	-
3	SIN	A	219	-	-	X	-
3	SIN	A	221	-	-	X	-
3	SIN	A	223	-	-	X	-
3	SIN	B	222	-	-	X	-
3	SIN	C	222	-	-	X	-
3	SIN	C	226	-	-	X	-
3	SIN	C	228	-	-	-	X
3	SIN	D	223	-	-	X	-
3	SIN	D	224	-	-	X	-
3	SIN	D	225	-	-	X	-
3	SIN	E	218	-	-	X	-
3	SIN	E	222	-	-	X	-
3	SIN	G	218	-	-	X	-
3	SIN	H	219	-	-	X	-
3	SIN	H	222	-	-	-	X
4	MLI	A	225	-	-	-	X
4	MLI	B	225	-	-	X	X
4	MLI	C	231	-	-	X	-
4	MLI	C	232	-	-	-	X
4	MLI	D	226	-	-	X	-
4	MLI	D	227	-	-	X	-
4	MLI	D	228	-	-	X	-
4	MLI	E	223	-	-	X	-
4	MLI	F	224	-	-	X	-
5	CL	C	235	-	-	X	-
5	CL	C	236	-	-	X	-
5	CL	D	230	-	-	X	-
6	FLC	B	218	-	-	X	X
6	FLC	F	218	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 15104 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 Oxygen-insensitive NAD(P)H nitroreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	219	Total 1715	C 1083	N 291	O 334	S 1	Se 6	0	3	0
1	B	219	Total 1713	C 1082	N 293	O 331	S 1	Se 6	0	3	0
1	C	218	Total 1698	C 1073	N 289	O 329	S 1	Se 6	0	1	0
1	D	219	Total 1720	C 1089	N 292	O 332	S 1	Se 6	0	3	0
1	E	219	Total 1700	C 1073	N 291	O 329	S 1	Se 6	0	0	0
1	F	219	Total 1705	C 1076	N 291	O 331	S 1	Se 6	0	1	0
1	G	218	Total 1698	C 1073	N 289	O 329	S 1	Se 6	0	1	0
1	H	220	Total 1725	C 1088	N 295	O 335	S 1	Se 6	0	3	0

There are 24 discrepancies between the modelled and reference sequences:

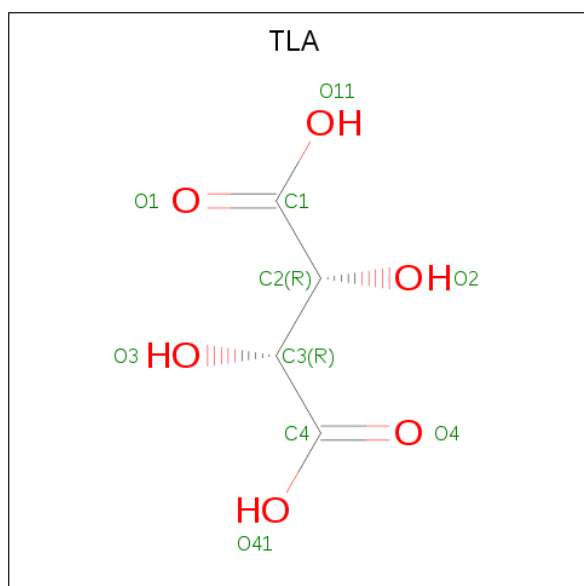
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P15888
A	-1	ASN	-	EXPRESSION TAG	UNP P15888
A	0	ALA	-	EXPRESSION TAG	UNP P15888
B	-2	SER	-	EXPRESSION TAG	UNP P15888
B	-1	ASN	-	EXPRESSION TAG	UNP P15888
B	0	ALA	-	EXPRESSION TAG	UNP P15888
C	-2	SER	-	EXPRESSION TAG	UNP P15888
C	-1	ASN	-	EXPRESSION TAG	UNP P15888
C	0	ALA	-	EXPRESSION TAG	UNP P15888
D	-2	SER	-	EXPRESSION TAG	UNP P15888
D	-1	ASN	-	EXPRESSION TAG	UNP P15888
D	0	ALA	-	EXPRESSION TAG	UNP P15888
E	-2	SER	-	EXPRESSION TAG	UNP P15888

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	ASN	-	EXPRESSION TAG	UNP P15888
E	0	ALA	-	EXPRESSION TAG	UNP P15888
F	-2	SER	-	EXPRESSION TAG	UNP P15888
F	-1	ASN	-	EXPRESSION TAG	UNP P15888
F	0	ALA	-	EXPRESSION TAG	UNP P15888
G	-2	SER	-	EXPRESSION TAG	UNP P15888
G	-1	ASN	-	EXPRESSION TAG	UNP P15888
G	0	ALA	-	EXPRESSION TAG	UNP P15888
H	-2	SER	-	EXPRESSION TAG	UNP P15888
H	-1	ASN	-	EXPRESSION TAG	UNP P15888
H	0	ALA	-	EXPRESSION TAG	UNP P15888

- Molecule 2 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



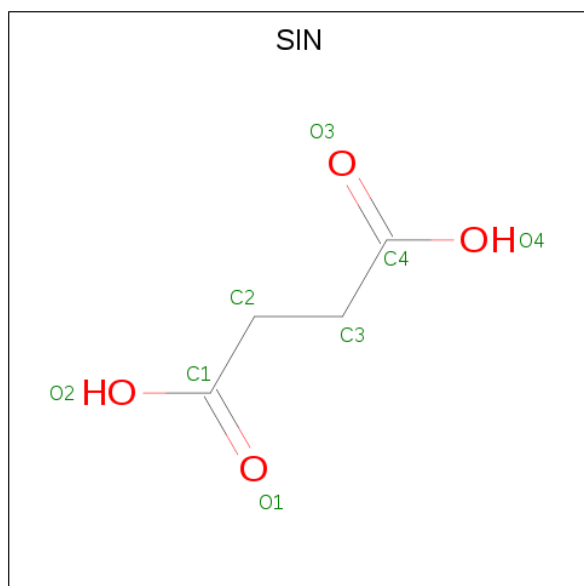
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 4 6	0	0
2	B	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	C	1	Total C O 10 4 6	0	0
2	D	1	Total C O 10 4 6	0	0
2	F	1	Total C O 10 4 6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄).



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

Continued on next page...

Continued from previous page...

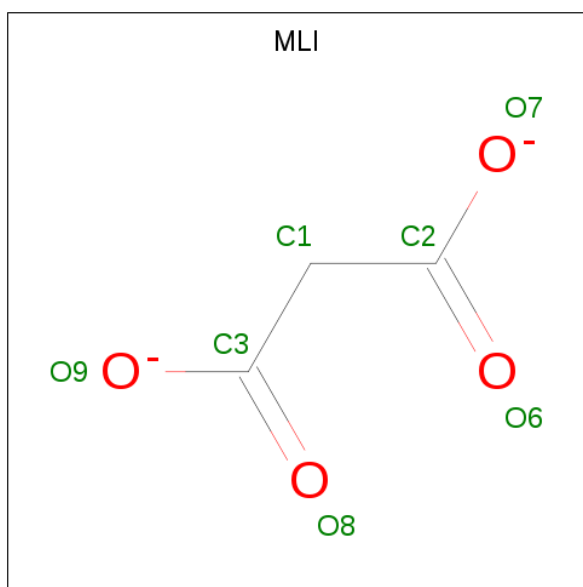
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	C	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	D	1	Total	C	O	0	0
			8	4	4		
3	E	1	Total	C	O	0	0
			8	4	4		
3	E	1	Total	C	O	0	0
			8	4	4		
3	E	1	Total	C	O	0	0
			8	4	4		
3	E	1	Total	C	O	0	0
			8	4	4		
3	E	1	Total	C	O	0	0
			8	4	4		
3	F	1	Total	C	O	0	0
			8	4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	C	O	0	0
			8	4	4		
3	F	1	Total	C	O	0	0
			8	4	4		
3	F	1	Total	C	O	0	0
			8	4	4		
3	G	1	Total	C	O	0	0
			8	4	4		
3	G	1	Total	C	O	0	0
			8	4	4		
3	G	1	Total	C	O	0	0
			8	4	4		
3	G	1	Total	C	O	0	0
			8	4	4		
3	H	1	Total	C	O	0	0
			8	4	4		
3	H	1	Total	C	O	0	0
			8	4	4		
3	H	1	Total	C	O	0	0
			8	4	4		
3	H	1	Total	C	O	0	0
			8	4	4		

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: C₃H₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	A	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0

Continued on next page...

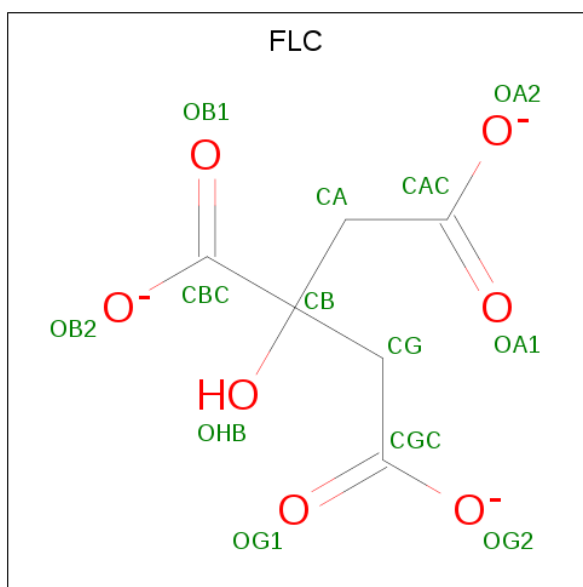
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			7	3	4		
4	F	1	Total	C	O	0	0
			7	3	4		
4	G	1	Total	C	O	0	0
			7	3	4		
4	G	1	Total	C	O	0	0
			7	3	4		
4	H	1	Total	C	O	0	0
			7	3	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		
5	D	2	Total	Cl	0	0
			2	2		
5	E	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		
5	C	4	Total	Cl	0	0
			4	4		
5	A	1	Total	Cl	0	0
			1	1		
5	F	1	Total	Cl	0	0
			1	1		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).

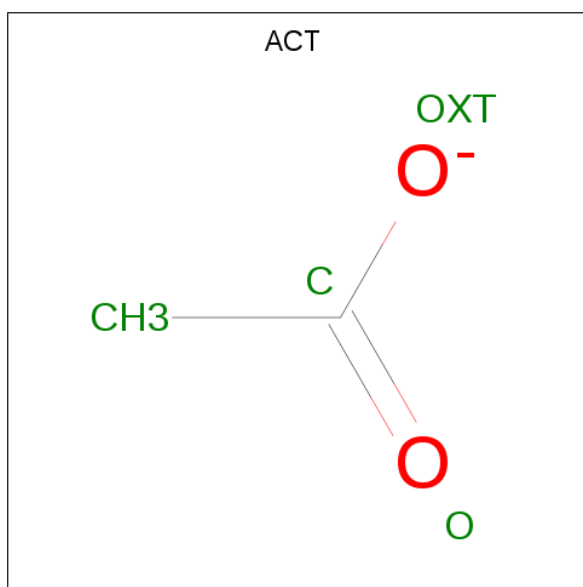


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 13 6 7	0	0
6	F	1	Total C O 13 6 7	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0
7	E	1	Total Na 1 1	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0
8	D	1	Total C O 4 2 2	0	0
8	G	1	Total C O 4 2 2	0	0

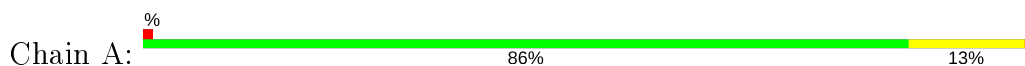
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	111	Total O 114 114	0	3
9	B	66	Total O 67 67	0	1
9	C	128	Total O 130 130	0	2
9	D	130	Total O 131 131	0	1
9	E	108	Total O 109 109	0	1
9	F	113	Total O 114 114	0	1
9	G	78	Total O 80 80	0	2
9	H	75	Total O 76 76	0	1

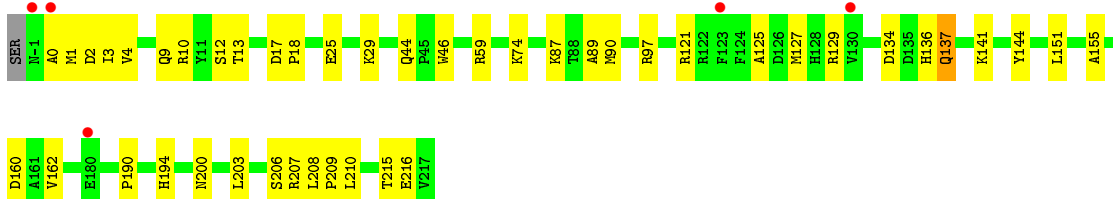
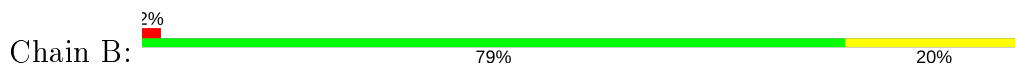
3 Residue-property plots [i](#)

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.

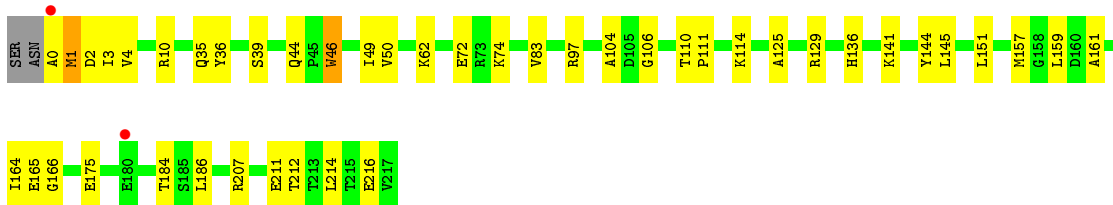
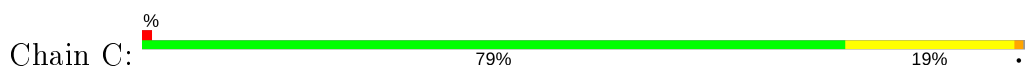
- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase



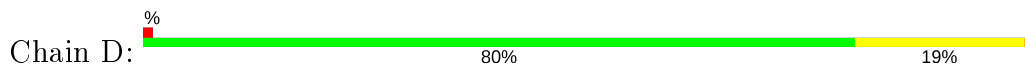
- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase



- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase

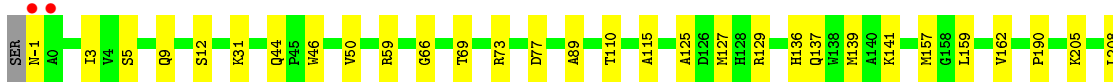
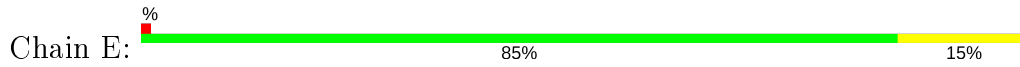


- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase

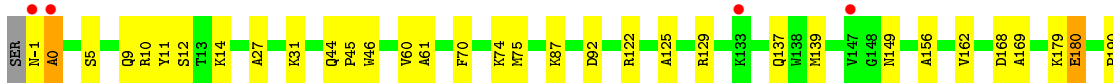
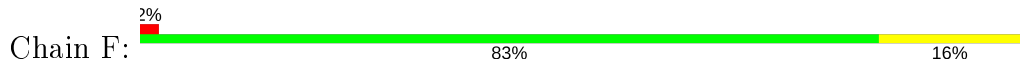




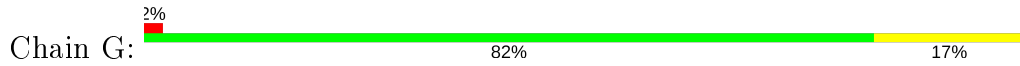
- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase



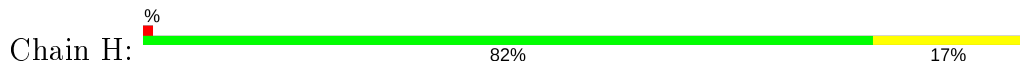
- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase



- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase



- Molecule 1: Oxygen-insensitive NAD(P)H nitroreductase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	280.34Å 96.76Å 131.84Å 90.00° 90.36° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.40) 99.0 (30.00-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.37 (at 2.39Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.177 , 0.222 0.177 , 0.219	Depositor DCC
R_{free} test set	6862 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15104	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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: CL, NA, MLI, TLA, ACT, FLC, SIN

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	0.48	0/1753	0.54	0/2362
1	B	0.44	0/1752	0.52	0/2361
1	C	0.53	0/1730	0.58	0/2331
1	D	0.50	0/1756	0.55	0/2366
1	E	0.48	0/1729	0.55	0/2330
1	F	0.47	0/1737	0.54	0/2341
1	G	0.45	0/1730	0.50	0/2331
1	H	0.42	0/1763	0.51	0/2375
All	All	0.47	0/13950	0.54	0/18797

There are no bond length outliers.

There are no bond angle outliers.

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	1715	0	1685	70	0
1	B	1713	0	1685	61	0
1	C	1698	0	1668	75	0
1	D	1720	0	1686	63	0
1	E	1700	0	1668	46	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1705	0	1672	71	0
1	G	1698	0	1668	43	0
1	H	1725	0	1696	54	0
2	A	10	0	4	1	0
2	B	10	0	4	0	0
2	C	20	0	8	0	0
2	D	10	0	4	0	0
2	F	10	0	4	1	0
2	H	10	0	4	4	0
3	A	48	0	24	33	0
3	B	24	0	12	9	0
3	C	72	0	36	28	0
3	D	56	0	28	24	0
3	E	40	0	20	14	0
3	F	32	0	16	3	0
3	G	40	0	20	10	0
3	H	40	0	20	13	0
4	A	28	0	8	0	0
4	B	21	0	6	7	0
4	C	28	0	8	10	0
4	D	21	0	6	7	0
4	E	7	0	2	7	0
4	F	7	0	2	5	0
4	G	14	0	4	2	0
4	H	7	0	2	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	4	0	0	4	0
5	D	2	0	0	3	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
6	B	13	0	5	5	0
6	F	13	0	5	19	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
8	C	4	0	3	0	0
8	D	4	0	3	0	0
8	G	4	0	3	0	0
9	A	114	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	67	0	0	2	0
9	C	130	0	0	4	0
9	D	131	0	0	5	0
9	E	109	0	0	0	0
9	F	114	0	0	10	0
9	G	80	0	0	4	0
9	H	76	0	0	6	0
All	All	15104	0	13689	455	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 16.

All (455) 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)
3:A:219:SIN:H21	1:B:137:GLN:CB	1.52	1.39
1:D:-1:ASN:N	1:D:156:ALA:HB1	1.38	1.32
1:D:10:ARG:HE	3:D:223:SIN:C2	1.46	1.29
1:F:61:ALA:HA	1:F:75:MSE:CE	1.64	1.25
1:D:60:VAL:HG12	1:D:75:MSE:CE	1.70	1.20
1:A:29:LYS:HE3	4:B:225:MLI:O8	1.41	1.19
1:F:87:LYS:HB2	1:F:139:MSE:CE	1.75	1.14
1:F:61:ALA:HA	1:F:75:MSE:HE2	1.20	1.13
1:E:141:LYS:NZ	3:E:222:SIN:H32	1.63	1.12
1:E:141:LYS:HZ1	3:E:222:SIN:H32	1.03	1.11
1:A:137:GLN:HB3	3:A:219:SIN:H32	1.13	1.11
1:D:10:ARG:HE	3:D:223:SIN:H22	1.12	1.11
1:H:74:LYS:HE2	3:H:219:SIN:O1	1.49	1.11
1:C:1:MSE:CG	1:C:2:ASP:HA	1.81	1.10
1:F:11:TYR:HA	6:F:218:FLC:CG	1.82	1.10
1:C:1:MSE:HG2	1:C:2:ASP:HA	1.10	1.09
1:F:11:TYR:HA	6:F:218:FLC:HG1	1.31	1.09
1:F:12:SER:H	6:F:218:FLC:CA	1.64	1.08
1:F:87:LYS:HB2	1:F:139:MSE:HE1	1.24	1.08
1:A:61:ALA:HA	1:A:75:MSE:CE	1.84	1.07
1:A:61:ALA:HA	1:A:75:MSE:HE2	1.08	1.07
1:C:10:ARG:HE	3:C:222:SIN:H31	0.96	1.07
1:C:1:MSE:HB2	1:C:3:ILE:N	1.70	1.07
1:C:114:LYS:HE2	3:C:226:SIN:H31	1.10	1.06
1:C:10:ARG:HE	3:C:222:SIN:C3	1.66	1.06
1:F:12:SER:H	6:F:218:FLC:HA1	1.10	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:12:SER:N	6:F:218:FLC:HA1	1.70	1.04
1:D:60:VAL:HG12	1:D:75:MSE:HE2	1.40	1.03
3:A:219:SIN:H21	1:B:137:GLN:HB2	1.09	1.03
1:A:61:ALA:CA	1:A:75:MSE:HE2	1.88	1.02
1:A:60:VAL:HG12	1:A:75:MSE:HE3	1.37	1.02
1:D:59:ARG:HH22	3:D:222:SIN:H31	1.16	1.02
1:C:114:LYS:HE2	3:C:226:SIN:C3	1.89	1.01
3:A:219:SIN:H21	1:B:137:GLN:HB3	1.42	1.01
1:D:10:ARG:HE	3:D:223:SIN:H21	1.24	1.01
1:C:10:ARG:NE	3:C:222:SIN:H31	1.74	1.01
3:E:218:SIN:H32	9:F:489:HOH:O	1.60	1.01
1:C:1:MSE:HB2	1:C:3:ILE:H	1.21	1.00
1:D:-1:ASN:H1	1:D:156:ALA:HB1	0.89	0.99
1:D:-1:ASN:N	1:D:156:ALA:CB	2.26	0.98
1:F:12:SER:N	6:F:218:FLC:HG2	1.78	0.97
1:D:10:ARG:NE	3:D:223:SIN:H22	1.80	0.97
3:A:219:SIN:C2	1:B:137:GLN:HB2	1.94	0.97
6:F:218:FLC:CGC	6:F:218:FLC:OB2	2.09	0.96
1:E:59:ARG:HH22	3:E:221:SIN:H21	1.28	0.96
3:A:219:SIN:O4	1:B:137:GLN:HB3	1.66	0.96
1:G:208:LEU:H	1:H:44:GLN:HE22	1.08	0.96
1:A:208:LEU:H	1:B:44:GLN:HE22	1.12	0.95
1:C:151:LEU:HD22	3:C:222:SIN:O4	1.67	0.94
1:C:136:HIS:HB2	3:C:223:SIN:O4	1.66	0.94
1:B:155:ALA:HB2	3:B:222:SIN:H31	1.48	0.93
1:D:60:VAL:HG12	1:D:75:MSE:HE1	1.47	0.93
1:E:44:GLN:HE22	1:F:208:LEU:H	1.15	0.93
1:D:10:ARG:NE	3:D:223:SIN:C2	2.30	0.93
1:C:1:MSE:CB	1:C:3:ILE:H	1.81	0.92
1:C:44:GLN:HE22	1:D:208:LEU:H	1.09	0.92
1:E:208:LEU:H	1:F:44:GLN:HE22	1.17	0.92
1:A:44:GLN:HE22	1:B:208:LEU:H	1.15	0.91
1:C:166:GLY:H	4:C:231:MLI:H11	1.34	0.91
1:D:10:ARG:HH21	3:D:223:SIN:C1	1.82	0.91
1:D:75:MSE:HE3	1:D:188:VAL:HG11	1.53	0.91
1:F:61:ALA:HA	1:F:75:MSE:HE1	1.52	0.89
1:H:33:LEU:CD1	1:H:157:MSE:HE3	2.03	0.89
1:C:166:GLY:N	4:C:231:MLI:H11	1.88	0.88
1:C:1:MSE:H	1:C:1:MSE:HE2	1.38	0.88
1:H:41:THR:HG21	1:H:121:ARG:HG3	1.54	0.87
1:C:114:LYS:CE	3:C:226:SIN:H31	2.03	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:LYS:CB	1:F:139:MSE:HE1	2.05	0.86
1:G:59:ARG:HH22	3:G:218:SIN:H31	1.38	0.86
1:F:61:ALA:CA	1:F:75:MSE:HE2	2.03	0.86
1:F:12:SER:H	6:F:218:FLC:HG2	1.39	0.86
1:A:59:ARG:HH22	3:A:220:SIN:H21	1.41	0.85
1:D:60:VAL:CG1	1:D:75:MSE:CE	2.53	0.85
1:E:141:LYS:NZ	3:E:222:SIN:C3	2.39	0.85
1:F:61:ALA:CA	1:F:75:MSE:CE	2.52	0.84
1:C:165:GLU:H	4:C:231:MLI:C1	1.90	0.84
6:B:218:FLC:OB1	6:B:218:FLC:CAC	2.25	0.84
5:C:235:CL:CL	5:D:231:CL:CL	2.70	0.84
1:A:29:LYS:CE	4:B:225:MLI:O8	2.24	0.83
4:E:223:MLI:H12	4:F:224:MLI:C2	2.08	0.83
1:E:59:ARG:HH22	3:E:221:SIN:C2	1.91	0.83
1:G:136:HIS:CE1	1:G:137:GLN:HE21	1.96	0.83
1:A:1:MSE:HA	9:A:755:HOH:O	1.76	0.82
3:A:219:SIN:C2	1:B:137:GLN:CB	2.48	0.82
1:H:33:LEU:CD1	1:H:157:MSE:CE	2.58	0.82
1:G:27:ALA:HB1	3:G:221:SIN:H21	1.62	0.82
1:E:31:LYS:HE2	1:F:216:GLU:OE2	1.78	0.81
1:C:106:GLY:HA3	3:C:228:SIN:H31	1.62	0.81
1:C:10:ARG:HH21	3:C:222:SIN:C4	1.93	0.81
1:F:87:LYS:HB2	1:F:139:MSE:HE2	1.63	0.81
1:G:44:GLN:HE22	1:H:208:LEU:H	1.29	0.80
3:H:219:SIN:H32	9:H:724:HOH:O	1.81	0.80
3:A:223:SIN:H31	9:A:775:HOH:O	1.81	0.80
3:D:224:SIN:H21	1:E:115:ALA:HB2	1.64	0.80
1:A:60:VAL:O	1:A:75:MSE:HE1	1.82	0.79
1:C:166:GLY:H	4:C:231:MLI:C1	1.94	0.79
3:D:219:SIN:H22	9:D:482:HOH:O	1.82	0.79
1:H:33:LEU:HD11	1:H:157:MSE:HE3	1.64	0.79
1:D:214:LEU:HD23	4:D:227:MLI:H12	1.66	0.77
9:A:804:HOH:O	1:B:127:MSE:HE1	1.84	0.77
1:A:136:HIS:ND1	1:A:137:GLN:HG3	1.99	0.77
1:E:59:ARG:NH2	3:E:221:SIN:H21	1.98	0.77
1:A:137:GLN:CB	3:A:219:SIN:H32	2.05	0.77
4:D:228:MLI:H11	9:D:759:HOH:O	1.84	0.77
1:F:11:TYR:HA	6:F:218:FLC:HG2	1.64	0.77
1:H:33:LEU:HD11	1:H:157:MSE:CE	2.15	0.76
1:A:141:LYS:CE	3:A:219:SIN:H31	2.15	0.76
1:D:151:LEU:HD22	3:D:223:SIN:O1	1.86	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:ASN:HD21	1:G:121:ARG:HH22	1.31	0.76
1:A:137:GLN:HB3	3:A:219:SIN:C3	2.06	0.75
1:B:134:ASP:HA	1:B:136[B]:HIS:CE1	2.21	0.75
1:B:10:ARG:HE	3:B:222:SIN:H32	1.50	0.75
1:D:199[B]:PHE:HD2	1:E:110:THR:HG22	1.51	0.75
1:F:11:TYR:CA	6:F:218:FLC:CG	2.62	0.74
4:E:223:MLI:C1	4:F:224:MLI:C2	2.65	0.74
1:C:62:LYS:HE2	1:C:175:GLU:OE1	1.87	0.74
1:C:1:MSE:CG	1:C:3:ILE:H	2.01	0.74
1:A:141:LYS:HE2	3:A:219:SIN:H31	1.68	0.74
1:C:74:LYS:HG3	9:C:271:HOH:O	1.88	0.74
1:D:59:ARG:NH2	3:D:222:SIN:H31	2.00	0.73
1:D:-1:ASN:H1	1:D:156:ALA:CB	1.84	0.73
4:E:223:MLI:H11	4:F:224:MLI:O7	1.90	0.72
1:C:165:GLU:H	4:C:231:MLI:H12	1.54	0.72
1:F:11:TYR:CA	6:F:218:FLC:HG2	2.19	0.72
1:B:10:ARG:HB2	3:B:222:SIN:H32	1.70	0.72
1:H:40:SER:O	1:H:41:THR:HB	1.89	0.72
1:H:33:LEU:HD12	1:H:157:MSE:HE3	1.71	0.71
1:H:74:LYS:N	3:H:219:SIN:O2	2.23	0.71
1:A:-1:ASN:HA	1:B:1:MSE:HA	1.72	0.71
1:A:111:PRO:HD3	3:A:223:SIN:H22	1.73	0.71
1:A:112:GLU:HA	3:H:219:SIN:O4	1.90	0.70
3:A:219:SIN:C4	1:B:137:GLN:HB3	2.21	0.70
3:C:226:SIN:H22	1:F:70:PHE:HA	1.72	0.70
4:D:226:MLI:O7	1:H:196:VAL:HG21	1.91	0.70
1:F:179:LYS:HB3	1:F:180:GLU:OE1	1.93	0.69
1:H:41:THR:CG2	1:H:41:THR:O	2.39	0.69
1:C:97:ARG:NH1	5:C:236:CL:CL	2.59	0.69
1:H:41:THR:O	1:H:41:THR:HG22	1.92	0.69
1:G:208:LEU:N	1:H:44:GLN:HE22	1.86	0.69
1:C:165:GLU:H	4:C:231:MLI:C2	2.05	0.69
1:G:87:LYS:HE3	1:G:94:TRP:CG	2.28	0.68
4:E:223:MLI:C1	4:F:224:MLI:O7	2.41	0.68
1:A:60:VAL:HG12	1:A:75:MSE:CE	2.20	0.67
1:C:165:GLU:N	4:C:231:MLI:H12	2.10	0.67
9:A:526:HOH:O	3:H:219:SIN:H31	1.95	0.67
1:H:73[A]:ARG:HB3	3:H:219:SIN:O2	1.94	0.67
4:C:232:MLI:H11	9:C:762:HOH:O	1.95	0.67
1:D:136:HIS:HA	4:D:226:MLI:O6	1.94	0.67
1:E:31:LYS:HD3	1:F:214:LEU:HD21	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:LEU:H	1:H:44:GLN:NE2	1.88	0.66
1:B:151:LEU:HD22	3:B:222:SIN:O2	1.95	0.66
1:E:141:LYS:HZ3	3:E:222:SIN:C3	2.06	0.66
1:D:10:ARG:NE	3:D:223:SIN:H21	2.02	0.66
1:C:1:MSE:HG3	1:C:3:ILE:H	1.60	0.65
1:F:12:SER:H	6:F:218:FLC:CG	2.09	0.65
1:H:73[B]:ARG:HB3	3:H:219:SIN:O2	1.96	0.65
1:B:1:MSE:O	4:B:225:MLI:H12	1.95	0.65
1:F:11:TYR:C	6:F:218:FLC:HG2	2.16	0.65
1:B:10:ARG:NE	3:B:222:SIN:H32	2.12	0.64
1:H:87:LYS:HE3	1:H:89:ALA:O	1.97	0.64
1:G:117:ASN:HB2	3:G:220:SIN:H21	1.78	0.64
1:A:47:HIS:HE1	1:B:215:THR:OG1	1.81	0.63
1:A:60:VAL:C	1:A:75:MSE:CE	2.67	0.63
1:A:208:LEU:H	1:B:44:GLN:NE2	1.92	0.63
1:E:31:LYS:HD3	1:F:214:LEU:CD2	2.28	0.63
1:D:7:ALA:O	5:D:230:CL:CL	2.54	0.63
1:D:199[B]:PHE:CD2	1:E:110:THR:HG22	2.32	0.63
1:A:61:ALA:CA	1:A:75:MSE:CE	2.64	0.63
1:C:184:THR:HG21	3:C:223:SIN:H22	1.79	0.62
1:H:74:LYS:CE	3:H:219:SIN:O1	2.38	0.62
1:A:141:LYS:HD3	1:B:144:TYR:CE1	2.34	0.62
1:D:60:VAL:CG1	1:D:75:MSE:HE1	2.24	0.62
1:G:59:ARG:NH2	3:G:218:SIN:H31	2.13	0.62
1:C:1:MSE:CB	1:C:2:ASP:HA	2.29	0.62
1:D:60:VAL:CG1	1:D:75:MSE:HE2	2.24	0.62
1:G:80:HIS:NE2	3:G:221:SIN:H32	2.15	0.62
1:G:47:HIS:HD2	9:G:229:HOH:O	1.82	0.62
1:C:1:MSE:CG	1:C:2:ASP:CA	2.71	0.62
1:F:169:ALA:H	3:F:223:SIN:H32	1.65	0.62
1:B:125:ALA:O	1:B:129:ARG:HG2	1.99	0.61
1:A:141:LYS:HE3	3:A:219:SIN:H31	1.83	0.61
1:E:12:SER:HB3	1:E:162:VAL:HG23	1.81	0.61
1:E:3:ILE:N	4:E:223:MLI:O7	2.29	0.61
4:G:223:MLI:H12	9:G:727:HOH:O	1.99	0.61
1:C:165:GLU:N	4:C:231:MLI:C1	2.61	0.61
1:F:60:VAL:HG12	1:F:75:MSE:HE3	1.84	0.60
1:A:208:LEU:N	1:B:44:GLN:HE22	1.93	0.60
1:F:125:ALA:O	1:F:129:ARG:HG2	2.02	0.60
1:A:60:VAL:CG1	1:A:75:MSE:HE3	2.24	0.60
1:B:10:ARG:HB2	3:B:222:SIN:C3	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:ASN:HA	3:H:219:SIN:O1	2.02	0.59
1:B:10:ARG:HE	3:B:222:SIN:C3	2.16	0.59
1:G:136:HIS:CD2	1:G:136:HIS:H	2.21	0.59
1:C:97:ARG:HD3	5:C:236:CL:CL	2.40	0.59
1:E:137:GLN:HG3	9:H:230:HOH:O	2.03	0.59
1:A:44:GLN:HE22	1:B:208:LEU:N	1.95	0.58
1:F:12:SER:N	6:F:218:FLC:CA	2.42	0.58
1:G:55[B]:GLU:HA	1:G:55[B]:GLU:OE1	2.02	0.58
1:C:1:MSE:CB	1:C:3:ILE:N	2.49	0.58
1:F:11:TYR:CA	6:F:218:FLC:HG1	2.19	0.58
1:G:38:PRO:HG2	1:G:145:LEU:HD21	1.86	0.58
3:A:224:SIN:O1	6:B:218:FLC:OB2	2.21	0.58
1:C:10:ARG:NE	3:C:222:SIN:C3	2.49	0.58
1:E:125:ALA:O	1:E:129:ARG:HG2	2.04	0.58
1:A:101:GLN:NE2	3:A:221:SIN:H31	2.19	0.57
1:H:40:SER:H	1:H:142:GLN:NE2	2.02	0.57
1:E:44:GLN:HE22	1:F:208:LEU:N	1.96	0.57
1:A:-1:ASN:HD22	1:B:1:MSE:HA	1.69	0.57
3:A:221:SIN:H21	1:B:208:LEU:CD2	2.35	0.57
1:D:80:HIS:NE2	3:D:225:SIN:H22	2.20	0.57
1:G:87:LYS:HE3	1:G:94:TRP:CD2	2.39	0.57
3:A:221:SIN:H21	1:B:208:LEU:HD22	1.86	0.57
4:E:223:MLI:O6	1:F:156:ALA:O	2.22	0.57
1:A:111:PRO:CD	3:A:223:SIN:H22	2.34	0.56
1:A:101:GLN:HE21	3:A:221:SIN:C3	2.17	0.56
1:A:101:GLN:HE21	3:A:221:SIN:C2	2.18	0.56
3:A:219:SIN:C2	1:B:137:GLN:HB3	2.27	0.56
1:G:90:MSE:O	1:G:129:ARG:HD3	2.06	0.56
1:A:-1:ASN:ND2	1:B:1:MSE:HG3	2.20	0.56
1:G:136:HIS:HE1	1:G:137:GLN:HE21	1.46	0.56
1:H:41:THR:CG2	1:H:121:ARG:HE	2.19	0.56
1:G:2:ASP:OD2	1:G:5:SER:HB2	2.06	0.56
1:C:1:MSE:H	1:C:1:MSE:CE	2.15	0.55
1:A:0:ALA:O	1:A:1:MSE:HB2	2.06	0.55
1:G:137:GLN:O	1:G:141:LYS:HG3	2.06	0.55
1:A:157:MSE:HG2	4:B:225:MLI:H11	1.87	0.55
1:A:-1:ASN:C	1:A:1:MSE:H	2.10	0.55
1:A:44:GLN:NE2	1:B:208:LEU:H	1.96	0.55
1:B:10:ARG:NH2	3:B:222:SIN:O1	2.31	0.55
1:C:1:MSE:CB	1:C:2:ASP:CA	2.85	0.55
1:C:4:VAL:HG21	1:D:29:LYS:HD2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ALA:O	3:C:222:SIN:O3	2.25	0.55
1:E:50:VAL:HG23	1:F:214:LEU:CD1	2.37	0.55
1:A:-1:ASN:H3	1:A:156:ALA:HB1	1.72	0.55
1:C:1:MSE:HE2	1:C:1:MSE:N	2.18	0.55
1:H:151:LEU:HB2	9:H:229:HOH:O	2.07	0.54
1:F:45:PRO:HB2	1:F:139:MSE:HE2	1.88	0.54
1:H:33:LEU:HD12	1:H:157:MSE:CE	2.33	0.54
1:A:60:VAL:O	1:A:75:MSE:CE	2.53	0.54
1:H:91:ASP:N	1:H:91:ASP:OD1	2.36	0.54
1:B:210:LEU:HB2	6:B:218:FLC:OG1	2.08	0.54
1:A:61:ALA:N	1:A:75:MSE:HE2	2.23	0.54
1:A:31:LYS:NZ	1:B:216:GLU:OE2	2.31	0.54
1:H:41:THR:CG2	1:H:121:ARG:HG3	2.33	0.54
1:C:1:MSE:CG	1:C:3:ILE:N	2.71	0.54
1:A:117:ASN:HD21	1:A:121:ARG:HH22	1.54	0.54
1:F:60:VAL:O	1:F:75:MSE:HE1	2.08	0.54
1:C:151:LEU:O	3:C:222:SIN:H21	2.08	0.53
1:E:136:HIS:HB2	9:H:230:HOH:O	2.08	0.53
1:A:101:GLN:HE21	3:A:221:SIN:H22	1.73	0.53
1:F:169:ALA:H	3:F:223:SIN:C3	2.22	0.53
1:B:59:ARG:HH22	3:B:220:SIN:H22	1.74	0.53
1:C:106:GLY:CA	3:C:228:SIN:H31	2.34	0.53
1:E:50:VAL:CG2	1:F:214:LEU:HD11	2.39	0.53
4:E:223:MLI:H11	4:F:224:MLI:C2	2.36	0.53
4:D:227:MLI:O7	4:D:227:MLI:O9	2.23	0.53
1:G:59:ARG:HH22	3:G:218:SIN:C3	2.18	0.53
1:H:117:ASN:HD21	1:H:121:ARG:HH12	1.55	0.53
1:G:44:GLN:HE22	1:H:208:LEU:N	2.03	0.53
1:F:12:SER:HB2	6:F:218:FLC:HA2	1.90	0.52
1:H:125:ALA:O	1:H:129:ARG:HG2	2.09	0.52
4:D:228:MLI:C2	9:D:363:HOH:O	2.58	0.52
1:A:99:VAL:HG23	1:A:117:ASN:HD22	1.74	0.52
1:B:3:ILE:N	4:B:225:MLI:O9	2.42	0.52
1:A:4:VAL:HG21	1:B:29:LYS:HD2	1.92	0.52
1:D:40:SER:H	1:D:142:GLN:NE2	2.08	0.52
1:H:74:LYS:NZ	9:H:713:HOH:O	2.43	0.51
1:C:36:TYR:O	5:D:230:CL:CL	2.65	0.51
1:G:27:ALA:O	1:G:31:LYS:HD3	2.10	0.51
1:H:2:ASP:CG	1:H:5:SER:HB2	2.31	0.51
1:H:41:THR:CG2	1:H:121:ARG:NE	2.74	0.51
1:A:117:ASN:ND2	1:A:121:ARG:HH12	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:THR:OG1	1:H:47:HIS:HE1	1.94	0.51
1:E:141:LYS:HZ3	3:E:222:SIN:H31	1.75	0.51
1:F:92[A]:ASP:OD1	1:F:122:ARG:NH2	2.42	0.51
1:C:1:MSE:HG3	1:C:3:ILE:N	2.25	0.51
1:D:87:LYS:HE2	1:D:94:TRP:CG	2.46	0.51
1:C:164:ILE:HA	4:C:231:MLI:H12	1.93	0.50
1:E:216:GLU:OE2	1:F:31:LYS:HE2	2.11	0.50
4:G:224:MLI:O7	4:G:224:MLI:O9	2.26	0.50
1:C:144:TYR:CE1	1:D:141:LYS:HD3	2.47	0.50
1:E:141:LYS:HE3	3:E:222:SIN:O2	2.11	0.50
1:C:44:GLN:NE2	1:D:208:LEU:H	1.93	0.50
1:D:63:SER:HB3	1:D:172:LEU:HB2	1.93	0.50
1:C:141:LYS:HE3	1:D:137[A]:GLN:HE22	1.77	0.50
1:G:195:SER:HB2	9:G:233:HOH:O	2.12	0.50
1:D:-1:ASN:H2	1:D:156:ALA:HB1	1.62	0.50
3:A:224:SIN:O1	6:B:218:FLC:CBC	2.60	0.50
1:G:117:ASN:HD21	1:G:121:ARG:NH2	2.07	0.49
1:A:61:ALA:N	1:A:75:MSE:CE	2.75	0.49
1:G:0:ALA:O	1:H:1:MSE:HE2	2.12	0.49
1:G:168:ASP:CG	1:G:171:VAL:HG23	2.32	0.49
1:G:27:ALA:CB	3:G:221:SIN:H21	2.39	0.49
1:B:200:ASN:HA	1:B:203:LEU:HD12	1.94	0.49
1:C:1:MSE:HA	1:D:-1:ASN:HA	1.95	0.49
1:A:136:HIS:CE1	1:A:137:GLN:HG3	2.47	0.49
1:H:41:THR:HG22	1:H:121:ARG:HE	1.78	0.49
1:H:92[B]:ASP:OD1	1:H:122:ARG:NH2	2.39	0.49
1:C:184:THR:HG21	3:C:223:SIN:C2	2.42	0.49
1:F:-1:ASN:O	1:F:0:ALA:HB2	2.13	0.49
1:A:112:GLU:CA	3:H:219:SIN:O4	2.59	0.48
1:D:199[B]:PHE:HD2	1:E:110:THR:CG2	2.24	0.48
3:C:226:SIN:C2	1:F:70:PHE:HA	2.43	0.48
1:H:25:GLU:HB3	3:H:222:SIN:H22	1.96	0.48
1:H:70:PHE:O	3:H:219:SIN:C1	2.61	0.48
1:A:0:ALA:HB3	1:B:0:ALA:HB3	1.95	0.48
1:C:0:ALA:HA	1:C:1:MSE:HE2	1.96	0.48
1:F:61:ALA:CA	1:F:75:MSE:HE1	2.32	0.48
1:G:49:ILE:HB	1:G:83:VAL:HB	1.94	0.48
1:B:25:GLU:O	1:B:29:LYS:HG2	2.14	0.48
1:D:145:LEU:C	1:D:145:LEU:HD23	2.34	0.48
1:F:196:VAL:HG23	9:F:462:HOH:O	2.13	0.48
1:H:70:PHE:O	3:H:219:SIN:C2	2.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLN:HE21	3:A:221:SIN:H31	1.79	0.47
1:E:31:LYS:CE	9:F:627:HOH:O	2.61	0.47
1:F:92[A]:ASP:OD1	1:F:122:ARG:NH1	2.46	0.47
1:E:44:GLN:NE2	1:F:208:LEU:H	1.97	0.47
1:C:50:VAL:HG23	1:D:214:LEU:HD11	1.97	0.47
1:C:1:MSE:C	1:D:-1:ASN:HA	2.34	0.47
1:G:176:PHE:HA	3:G:218:SIN:H22	1.95	0.47
3:E:222:SIN:O1	1:F:137:GLN:HG2	2.14	0.47
1:E:5:SER:O	1:E:9:GLN:HG2	2.14	0.47
1:G:44:GLN:NE2	1:H:208:LEU:H	2.05	0.47
1:B:87:LYS:HE3	1:B:89:ALA:O	2.14	0.47
1:F:180:GLU:CD	1:F:180:GLU:H	2.18	0.47
1:H:117:ASN:ND2	1:H:121:ARG:HH12	2.13	0.47
1:A:111:PRO:HD3	3:A:223:SIN:C2	2.43	0.47
1:D:136:HIS:HB3	4:D:226:MLI:O8	2.15	0.47
1:C:161:ALA:HB3	3:C:222:SIN:H22	1.96	0.46
1:A:-1:ASN:CA	1:B:1:MSE:HA	2.44	0.46
1:C:159:LEU:O	3:C:222:SIN:O1	2.34	0.46
3:D:225:SIN:H32	9:D:461:HOH:O	2.15	0.46
1:E:214:LEU:HD21	1:F:31:LYS:HD3	1.97	0.46
1:G:141:LYS:HD3	1:H:144:TYR:CE2	2.50	0.46
1:E:50:VAL:HG23	1:F:214:LEU:HD11	1.96	0.46
1:D:45:PRO:HA	1:D:87:LYS:HD3	1.97	0.46
1:G:12:SER:HB3	1:G:162:VAL:HG23	1.98	0.46
1:D:80:HIS:NE2	3:D:225:SIN:C2	2.78	0.46
1:A:-1:ASN:H1	1:B:1:MSE:HA	1.80	0.46
1:C:1:MSE:HG3	9:C:756:HOH:O	2.16	0.46
1:F:74:LYS:NZ	2:F:219:TLA:O3	2.49	0.46
1:F:45:PRO:HB2	1:F:139:MSE:CE	2.45	0.46
1:C:157:MSE:HB3	3:C:225:SIN:H21	1.98	0.46
1:D:161:ALA:HB3	3:D:223:SIN:H31	1.97	0.46
1:G:124:PHE:CZ	2:H:218:TLA:H2	2.50	0.46
1:H:47:HIS:HD2	9:H:236:HOH:O	1.99	0.46
1:E:157:MSE:HE2	1:E:159:LEU:HD11	1.97	0.45
1:H:5:SER:O	1:H:9:GLN:HG2	2.16	0.45
1:D:90:MSE:HE2	1:D:139:MSE:SE	2.66	0.45
1:E:31:LYS:HE3	9:F:627:HOH:O	2.15	0.45
1:F:45:PRO:HB3	1:F:139:MSE:HE3	1.99	0.45
1:F:12:SER:HB3	1:F:162:VAL:HG23	1.98	0.45
1:D:161:ALA:O	3:D:223:SIN:O2	2.35	0.45
1:E:89:ALA:CA	1:E:139:MSE:HE1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:GLN:HG3	9:F:809:HOH:O	2.16	0.45
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.81	0.45
1:C:207:ARG:NH1	5:C:235:CL:CL	2.87	0.45
1:E:127:MSE:CE	9:F:298:HOH:O	2.64	0.45
1:A:2:ASP:N	9:A:755:HOH:O	2.50	0.45
1:B:121:ARG:HD2	9:B:234:HOH:O	2.17	0.45
1:D:10:ARG:O	1:D:205:LYS:HE2	2.17	0.45
1:E:136:HIS:N	1:E:136:HIS:CD2	2.84	0.45
1:H:162:VAL:O	1:H:190:PRO:HD2	2.17	0.45
1:A:29:LYS:HE3	4:B:225:MLI:C3	2.35	0.44
1:A:29:LYS:HG2	1:B:4:VAL:HG21	2.00	0.44
1:G:217:VAL:OXT	1:H:53:THR:OG1	2.27	0.44
1:A:59:ARG:NH2	3:A:220:SIN:H21	2.21	0.44
3:D:224:SIN:C2	1:E:115:ALA:HB2	2.40	0.44
1:E:127:MSE:HE1	9:F:298:HOH:O	2.17	0.44
1:B:2:ASP:HA	4:B:225:MLI:O9	2.18	0.44
1:C:212:THR:HG23	3:C:227:SIN:H32	1.99	0.44
1:H:33:LEU:HD11	1:H:157:MSE:HE2	1.97	0.44
1:E:208:LEU:H	1:F:44:GLN:NE2	1.99	0.44
1:F:27:ALA:O	1:F:31:LYS:HG3	2.17	0.44
2:A:218:TLA:O1	2:A:218:TLA:O3	2.31	0.44
3:C:225:SIN:O2	1:D:1:MSE:O	2.34	0.44
1:D:74:LYS:HE3	3:D:224:SIN:O3	2.17	0.44
1:B:162:VAL:O	1:B:190:PRO:HD2	2.17	0.43
1:D:14:LYS:HB3	3:D:224:SIN:O4	2.18	0.43
1:B:137:GLN:O	1:B:141:LYS:HG3	2.17	0.43
1:E:214:LEU:CD2	1:F:31:LYS:HD3	2.48	0.43
1:A:137:GLN:O	1:A:141:LYS:HG3	2.18	0.43
1:D:151:LEU:HD13	3:D:223:SIN:O1	2.18	0.43
9:C:757:HOH:O	1:D:123:PHE:HE2	2.00	0.43
1:E:162:VAL:O	1:E:190:PRO:HD2	2.18	0.43
1:F:45:PRO:CB	1:F:139:MSE:HE3	2.48	0.43
1:H:17:ASP:OD1	1:H:19:SER:HB2	2.17	0.43
1:A:101:GLN:NE2	3:A:221:SIN:H22	2.33	0.43
1:D:88:THR:O	1:D:136:HIS:CE1	2.71	0.43
1:C:10:ARG:CZ	3:C:222:SIN:H31	2.42	0.43
1:C:72:GLU:OE2	3:C:221:SIN:H31	2.18	0.43
1:F:10:ARG:HH12	6:F:218:FLC:CGC	2.31	0.43
1:G:0:ALA:HB2	1:H:-2:SER:OG	2.19	0.43
1:A:97:ARG:HD3	3:A:221:SIN:O1	2.19	0.43
1:D:88:THR:O	1:D:136:HIS:HE1	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLU:HG2	3:D:225:SIN:O4	2.19	0.42
1:H:164:ILE:HA	2:H:218:TLA:O1	2.19	0.42
3:E:218:SIN:H31	9:F:733:HOH:O	2.18	0.42
1:A:136:HIS:ND1	1:A:137:GLN:N	2.66	0.42
1:G:113:ALA:O	3:G:220:SIN:O2	2.38	0.42
1:B:137:GLN:HG2	1:B:137:GLN:H	1.58	0.42
3:E:218:SIN:H21	9:F:460:HOH:O	2.18	0.42
1:F:45:PRO:CB	1:F:139:MSE:CE	2.98	0.42
1:D:50:VAL:HG22	1:D:82:VAL:HG22	2.02	0.42
1:H:41:THR:HG21	1:H:121:ARG:CG	2.39	0.42
1:B:74:LYS:HG3	9:B:237:HOH:O	2.18	0.42
1:C:104:ALA:O	3:C:228:SIN:O2	2.37	0.42
1:F:149:ASN:HB2	9:F:231:HOH:O	2.19	0.42
1:A:-1:ASN:N	1:A:156:ALA:HB1	2.34	0.42
1:B:209:PRO:HA	6:B:218:FLC:OHB	2.19	0.42
1:C:110:THR:HB	1:C:111:PRO:CD	2.50	0.42
1:C:214:LEU:CD2	1:D:31:LYS:HD3	2.50	0.42
1:E:136:HIS:CD2	1:E:136:HIS:H	2.37	0.42
1:C:10:ARG:HH21	3:C:222:SIN:C3	2.32	0.42
1:F:61:ALA:N	1:F:75:MSE:CE	2.83	0.42
1:G:47:HIS:CD2	9:G:229:HOH:O	2.65	0.42
1:C:186:LEU:O	3:C:224:SIN:O4	2.37	0.42
1:A:10:ARG:HG3	1:A:10:ARG:NH1	2.35	0.41
1:C:49:ILE:HB	1:C:83:VAL:HB	2.02	0.41
1:G:59:ARG:HH12	3:G:218:SIN:H31	1.84	0.41
1:F:168:ASP:HA	3:F:223:SIN:C3	2.50	0.41
1:C:35:GLN:HG3	9:D:236:HOH:O	2.21	0.41
1:E:73:ARG:HD3	1:E:77:ASP:OD1	2.21	0.41
1:F:162:VAL:O	1:F:190:PRO:HD2	2.19	0.41
1:B:90:MSE:O	1:B:129:ARG:NH1	2.54	0.41
1:G:136:HIS:CD2	1:G:136:HIS:N	2.88	0.41
1:A:101:GLN:CA	3:A:221:SIN:O3	2.69	0.41
1:B:160:ASP:OD2	1:B:194:HIS:HD2	2.04	0.41
1:C:39:SER:HB3	1:C:46:TRP:CH2	2.56	0.41
1:D:26:GLU:O	1:D:30:ILE:HG23	2.20	0.41
1:E:205:LYS:NZ	3:E:218:SIN:O4	2.54	0.41
1:F:12:SER:CB	6:F:218:FLC:HA2	2.48	0.41
1:E:66:GLY:O	1:E:69:THR:HG23	2.20	0.41
1:G:86:ALA:HB2	1:G:143:VAL:HG21	2.03	0.41
1:D:145:LEU:HD23	1:D:145:LEU:O	2.20	0.41
1:D:10:ARG:NH2	3:D:223:SIN:C1	2.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:THR:OG1	1:H:160:ASP:HB3	2.21	0.41
1:B:12:SER:HB3	1:B:162:VAL:HG23	2.03	0.41
1:C:145:LEU:HD23	1:C:145:LEU:C	2.42	0.41
1:D:200:ASN:N	1:D:200:ASN:HD22	2.19	0.41
3:A:219:SIN:C1	1:B:141:LYS:HE3	2.51	0.41
1:B:17:ASP:HA	1:B:18:PRO:HD3	1.92	0.41
1:B:206:SER:O	1:B:207:ARG:HD3	2.21	0.40
9:A:250:HOH:O	1:B:97:ARG:HD3	2.20	0.40
1:D:6:VAL:HA	3:D:221:SIN:H22	2.03	0.40
1:F:14:LYS:HE2	6:F:218:FLC:OA2	2.21	0.40
1:H:95:LEU:HD13	1:H:122:ARG:HG2	2.02	0.40
2:H:218:TLA:C1	2:H:218:TLA:O4	2.69	0.40
1:C:125:ALA:O	1:C:129:ARG:HG2	2.21	0.40
1:C:1:MSE:CA	1:D:-1:ASN:HA	2.51	0.40
1:B:13:THR:OG1	1:B:160:ASP:HB3	2.22	0.40
1:F:180:GLU:OE1	1:F:180:GLU:N	2.55	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	220/220 (100%)	211 (96%)	7 (3%)	2 (1%)	17	25
1	B	220/220 (100%)	216 (98%)	4 (2%)	0	100	100
1	C	217/220 (99%)	215 (99%)	2 (1%)	0	100	100
1	D	220/220 (100%)	215 (98%)	4 (2%)	1 (0%)	29	41
1	E	217/220 (99%)	212 (98%)	5 (2%)	0	100	100
1	F	218/220 (99%)	215 (99%)	2 (1%)	1 (0%)	29	41
1	G	217/220 (99%)	211 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	221/220 (100%)	215 (97%)	6 (3%)	0	100	100
All	All	1750/1760 (99%)	1710 (98%)	36 (2%)	4 (0%)	47	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	0	ALA
1	A	0	ALA
1	A	1	MSE
1	D	1	MSE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/175 (105%)	181 (99%)	2 (1%)	73	87
1	B	183/175 (105%)	181 (99%)	2 (1%)	73	87
1	C	180/175 (103%)	177 (98%)	3 (2%)	60	78
1	D	182/175 (104%)	179 (98%)	3 (2%)	62	79
1	E	180/175 (103%)	178 (99%)	2 (1%)	73	87
1	F	181/175 (103%)	178 (98%)	3 (2%)	60	78
1	G	180/175 (103%)	178 (99%)	2 (1%)	73	87
1	H	184/175 (105%)	181 (98%)	3 (2%)	62	79
All	All	1453/1400 (104%)	1433 (99%)	20 (1%)	67	82

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	TRP
1	A	74	LYS
1	B	46	TRP
1	B	137	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1	MSE
1	C	46	TRP
1	C	211	GLU
1	D	46	TRP
1	D	131	SER
1	D	205	LYS
1	E	-1	ASN
1	E	46	TRP
1	F	5	SER
1	F	46	TRP
1	F	180	GLU
1	G	46	TRP
1	G	216	GLU
1	H	46	TRP
1	H	91	ASP
1	H	117	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-1	ASN
1	A	44	GLN
1	A	47	HIS
1	A	101	GLN
1	A	117	ASN
1	A	137	GLN
1	B	44	GLN
1	B	149	ASN
1	B	194	HIS
1	C	44	GLN
1	C	101	GLN
1	D	9	GLN
1	D	71	ASN
1	D	142	GLN
1	D	200	ASN
1	E	-1	ASN
1	E	35	GLN
1	E	44	GLN
1	E	136	HIS
1	E	149	ASN
1	F	9	GLN
1	F	35	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	44	GLN
1	F	200	ASN
1	G	44	GLN
1	G	47	HIS
1	G	117	ASN
1	G	136	HIS
1	H	44	GLN
1	H	47	HIS
1	H	117	ASN
1	H	142	GLN
1	H	200	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](#)

Of 91 ligands modelled in this entry, 16 are monoatomic - leaving 75 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TLA	C	218	-	3,9,9	0.44	0	6,12,12	0.78	0
4	MLI	G	223	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	C	226	-	1,7,7	0.26	0	2,8,8	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLI	A	227	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	223	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	D	223	-	1,7,7	0.17	0	2,8,8	1.38	0
4	MLI	F	224	-	0,6,6	0.00	-	0,7,7	0.00	-
8	ACT	G	225	-	1,3,3	1.89	0	0,3,3	0.00	-
6	FLC	F	218	-	3,12,12	1.24	0	3,17,17	0.61	0
3	SIN	H	219	-	1,7,7	0.16	0	2,8,8	1.34	0
3	SIN	D	224	-	1,7,7	0.08	0	2,8,8	1.94	1 (50%)
3	SIN	A	223	-	1,7,7	0.13	0	2,8,8	1.87	1 (50%)
4	MLI	C	231	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	F	221	-	1,7,7	0.05	0	2,8,8	1.35	0
3	SIN	H	222	-	1,7,7	0.07	0	2,8,8	1.46	0
3	SIN	E	219	-	1,7,7	0.13	0	2,8,8	0.92	0
4	MLI	D	226	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	A	224	-	1,7,7	0.14	0	2,8,8	2.47	1 (50%)
3	SIN	G	218	-	1,7,7	0.08	0	2,8,8	1.68	0
4	MLI	A	228	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	C	223	-	1,7,7	0.01	0	2,8,8	0.83	0
3	SIN	G	219	-	1,7,7	0.09	0	2,8,8	0.89	0
4	MLI	A	226	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	224	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	A	222	-	1,7,7	0.02	0	2,8,8	0.90	0
3	SIN	G	221	-	1,7,7	0.12	0	2,8,8	2.33	1 (50%)
3	SIN	D	225	-	1,7,7	0.07	0	2,8,8	1.27	0
3	SIN	D	220	-	1,7,7	0.01	0	2,8,8	1.24	0
8	ACT	C	233	-	1,3,3	1.32	0	0,3,3	0.00	-
2	TLA	C	219	-	3,9,9	0.42	0	6,12,12	0.72	0
3	SIN	D	219	-	1,7,7	0.08	0	2,8,8	1.84	1 (50%)
3	SIN	G	220	-	1,7,7	0.29	0	2,8,8	4.06	2 (100%)
4	MLI	C	230	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	D	227	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	C	227	-	1,7,7	0.03	0	2,8,8	0.62	0
4	MLI	H	224	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	H	220	-	1,7,7	0.05	0	2,8,8	1.10	0
3	SIN	C	228	-	1,7,7	0.05	0	2,8,8	0.88	0
3	SIN	C	222	-	1,7,7	0.21	0	2,8,8	0.74	0
3	SIN	E	222	-	1,7,7	0.05	0	2,8,8	0.52	0
3	SIN	B	220	-	1,7,7	0.10	0	2,8,8	1.39	0
3	SIN	C	225	-	1,7,7	0.15	0	2,8,8	2.20	1 (50%)
2	TLA	F	219	-	3,9,9	0.56	0	6,12,12	0.93	0
3	SIN	E	221	-	1,7,7	0.11	0	2,8,8	1.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MLI	C	229	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	A	225	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	225	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	B	221	-	1,7,7	0.16	0	2,8,8	1.11	0
3	SIN	A	220	-	1,7,7	0.01	0	2,8,8	0.71	0
3	SIN	C	224	-	1,7,7	0.08	0	2,8,8	1.18	0
3	SIN	F	223	-	1,7,7	0.10	0	2,8,8	1.53	1 (50%)
3	SIN	B	222	-	1,7,7	0.05	0	2,8,8	0.80	0
3	SIN	C	220	-	1,7,7	0.16	0	2,8,8	1.31	0
3	SIN	E	218	-	1,7,7	0.21	0	2,8,8	2.52	2 (100%)
4	MLI	C	232	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	D	228	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	G	222	-	1,7,7	0.10	0	2,8,8	2.51	1 (50%)
4	MLI	E	223	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	F	220	-	1,7,7	0.14	0	2,8,8	0.71	0
6	FLC	B	218	-	3,12,12	1.21	0	3,17,17	1.63	1 (33%)
3	SIN	H	221	-	1,7,7	0.04	0	2,8,8	0.93	0
3	SIN	D	221	-	1,7,7	0.01	0	2,8,8	2.61	1 (50%)
3	SIN	A	219	-	1,7,7	0.08	0	2,8,8	0.89	0
2	TLA	H	218	-	3,9,9	0.38	0	6,12,12	1.79	1 (16%)
8	ACT	D	229	-	1,3,3	2.41	1 (100%)	0,3,3	0.00	-
2	TLA	B	219	-	3,9,9	0.48	0	6,12,12	1.56	2 (33%)
3	SIN	C	221	-	1,7,7	0.06	0	2,8,8	1.11	0
3	SIN	E	220	-	1,7,7	0.10	0	2,8,8	0.95	0
3	SIN	A	221	-	1,7,7	0.30	0	2,8,8	2.44	1 (50%)
2	TLA	A	218	-	3,9,9	0.36	0	6,12,12	0.82	0
3	SIN	D	222	-	1,7,7	0.05	0	2,8,8	0.84	0
4	MLI	G	224	-	0,6,6	0.00	-	0,7,7	0.00	-
3	SIN	F	222	-	1,7,7	0.01	0	2,8,8	1.07	0
2	TLA	D	218	-	3,9,9	0.74	0	6,12,12	1.38	2 (33%)
3	SIN	H	223	-	1,7,7	0.07	0	2,8,8	1.66	1 (50%)

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	TLA	C	218	-	-	0/4/12/12	-
4	MLI	G	223	-	-	0/0/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SIN	C	226	-	-	1/1/5/5	-
4	MLI	A	227	-	-	0/0/4/4	-
4	MLI	B	223	-	-	0/0/4/4	-
3	SIN	D	223	-	-	1/1/5/5	-
4	MLI	F	224	-	-	0/0/4/4	-
4	MLI	D	226	-	-	0/0/4/4	-
6	FLC	F	218	-	-	6/6/16/16	-
3	SIN	H	219	-	-	1/1/5/5	-
3	SIN	D	224	-	-	1/1/5/5	-
3	SIN	A	223	-	-	0/1/5/5	-
4	MLI	C	231	-	-	0/0/4/4	-
3	SIN	F	221	-	-	0/1/5/5	-
3	SIN	H	222	-	-	1/1/5/5	-
3	SIN	E	219	-	-	0/1/5/5	-
3	SIN	G	218	-	-	1/1/5/5	-
4	MLI	A	228	-	-	0/0/4/4	-
3	SIN	C	223	-	-	1/1/5/5	-
3	SIN	G	219	-	-	0/1/5/5	-
4	MLI	A	226	-	-	0/0/4/4	-
4	MLI	B	224	-	-	0/0/4/4	-
3	SIN	A	222	-	-	1/1/5/5	-
3	SIN	G	221	-	-	1/1/5/5	-
3	SIN	D	225	-	-	1/1/5/5	-
3	SIN	D	220	-	-	0/1/5/5	-
3	SIN	E	220	-	-	0/1/5/5	-
2	TLA	C	219	-	-	4/4/12/12	-
3	SIN	D	219	-	-	0/1/5/5	-
3	SIN	G	220	-	-	0/1/5/5	-
4	MLI	C	230	-	-	0/0/4/4	-
4	MLI	D	227	-	-	0/0/4/4	-
3	SIN	C	227	-	-	1/1/5/5	-
4	MLI	H	224	-	-	0/0/4/4	-
3	SIN	H	220	-	-	1/1/5/5	-
3	SIN	C	228	-	-	0/1/5/5	-
3	SIN	C	222	-	-	1/1/5/5	-
3	SIN	E	222	-	-	1/1/5/5	-
3	SIN	B	220	-	-	0/1/5/5	-
3	SIN	C	225	-	-	1/1/5/5	-
2	TLA	F	219	-	-	0/4/12/12	-
3	SIN	E	221	-	-	1/1/5/5	-
4	MLI	C	229	-	-	0/0/4/4	-
4	MLI	A	225	-	-	0/0/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MLI	B	225	-	-	0/0/4/4	-
3	SIN	B	221	-	-	0/1/5/5	-
3	SIN	A	220	-	-	1/1/5/5	-
3	SIN	C	224	-	-	1/1/5/5	-
3	SIN	F	223	-	-	1/1/5/5	-
3	SIN	B	222	-	-	0/1/5/5	-
3	SIN	C	220	-	-	0/1/5/5	-
3	SIN	E	218	-	-	0/1/5/5	-
4	MLI	C	232	-	-	0/0/4/4	-
4	MLI	D	228	-	-	0/0/4/4	-
3	SIN	G	222	-	-	0/1/5/5	-
4	MLI	E	223	-	-	0/0/4/4	-
3	SIN	F	220	-	-	0/1/5/5	-
6	FLC	B	218	-	-	4/6/16/16	-
3	SIN	H	221	-	-	1/1/5/5	-
3	SIN	D	221	-	-	1/1/5/5	-
3	SIN	A	219	-	-	1/1/5/5	-
2	TLA	H	218	-	-	1/4/12/12	-
2	TLA	B	219	-	-	0/4/12/12	-
3	SIN	C	221	-	-	0/1/5/5	-
3	SIN	A	224	-	-	0/1/5/5	-
3	SIN	A	221	-	-	1/1/5/5	-
2	TLA	A	218	-	-	4/4/12/12	-
3	SIN	D	222	-	-	0/1/5/5	-
4	MLI	G	224	-	-	0/0/4/4	-
3	SIN	F	222	-	-	0/1/5/5	-
2	TLA	D	218	-	-	0/4/12/12	-
3	SIN	H	223	-	-	0/1/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	229	ACT	CH3-C	2.41	1.51	1.48

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	220	SIN	C2-C3-C4	-5.01	104.27	112.67
2	H	218	TLA	O2-C2-C1	-3.81	101.93	111.10
3	G	222	SIN	C3-C2-C1	-3.54	106.73	112.67
3	D	221	SIN	C3-C2-C1	-3.38	107.00	112.67
3	A	221	SIN	C3-C2-C1	-3.32	107.11	112.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	224	SIN	C2-C3-C4	-3.25	107.22	112.67
3	G	221	SIN	C3-C2-C1	-2.97	107.69	112.67
2	B	219	TLA	C1-C2-C3	-2.96	106.74	113.11
3	G	220	SIN	C3-C2-C1	-2.81	107.95	112.67
3	E	218	SIN	C2-C3-C4	-2.80	107.98	112.67
3	C	225	SIN	C2-C3-C4	-2.61	108.29	112.67
3	D	224	SIN	C3-C2-C1	-2.55	108.39	112.67
6	B	218	FLC	CB-CA-CAC	-2.45	111.07	114.98
3	A	223	SIN	C3-C2-C1	-2.37	108.69	112.67
3	E	218	SIN	C3-C2-C1	-2.22	108.95	112.67
2	B	219	TLA	C4-C3-C2	-2.19	108.39	113.11
2	D	218	TLA	C1-C2-C3	-2.16	108.45	113.11
2	D	218	TLA	C4-C3-C2	-2.13	108.51	113.11
3	H	223	SIN	C2-C3-C4	-2.12	109.11	112.67
3	D	219	SIN	C2-C3-C4	-2.07	109.20	112.67
3	F	223	SIN	C3-C2-C1	-2.04	109.25	112.67

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	218	FLC	CA-CB-CG-CGC
6	F	218	FLC	CBC-CB-CG-CGC
6	F	218	FLC	OHB-CB-CG-CGC
3	C	223	SIN	C1-C2-C3-C4
3	H	222	SIN	C1-C2-C3-C4
3	A	219	SIN	C1-C2-C3-C4
3	A	221	SIN	C1-C2-C3-C4
3	G	221	SIN	C1-C2-C3-C4
3	D	221	SIN	C1-C2-C3-C4
2	C	219	TLA	C1-C2-C3-O3
2	C	219	TLA	C1-C2-C3-C4
2	C	219	TLA	O2-C2-C3-C4
2	A	218	TLA	C1-C2-C3-C4
2	A	218	TLA	O2-C2-C3-O3
3	A	222	SIN	C1-C2-C3-C4
3	A	220	SIN	C1-C2-C3-C4
6	B	218	FLC	CBC-CB-CG-CGC
6	B	218	FLC	OHB-CB-CG-CGC
2	A	218	TLA	C1-C2-C3-O3
2	A	218	TLA	O2-C2-C3-C4
2	C	219	TLA	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	222	SIN	C1-C2-C3-C4
6	B	218	FLC	CA-CB-CG-CGC
3	D	225	SIN	C1-C2-C3-C4
3	E	221	SIN	C1-C2-C3-C4
6	F	218	FLC	CAC-CA-CB-CBC
6	B	218	FLC	CAC-CA-CB-CBC
2	H	218	TLA	O2-C2-C3-O3
3	G	218	SIN	C1-C2-C3-C4
3	H	220	SIN	C1-C2-C3-C4
3	C	225	SIN	C1-C2-C3-C4
3	F	223	SIN	C1-C2-C3-C4
3	C	227	SIN	C1-C2-C3-C4
3	H	221	SIN	C1-C2-C3-C4
3	H	219	SIN	C1-C2-C3-C4
3	D	223	SIN	C1-C2-C3-C4
3	C	226	SIN	C1-C2-C3-C4
6	F	218	FLC	CAC-CA-CB-CG
6	F	218	FLC	CAC-CA-CB-OHB
3	C	224	SIN	C1-C2-C3-C4
3	C	222	SIN	C1-C2-C3-C4
3	D	224	SIN	C1-C2-C3-C4

There are no ring outliers.

45 monomers are involved in 195 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	223	MLI	1	0
3	C	226	SIN	5	0
3	D	223	SIN	12	0
4	F	224	MLI	5	0
6	F	218	FLC	19	0
3	H	219	SIN	12	0
3	D	224	SIN	4	0
3	A	223	SIN	4	0
4	C	231	MLI	9	0
3	H	222	SIN	1	0
4	D	226	MLI	3	0
3	A	224	SIN	2	0
3	G	218	SIN	5	0
3	C	223	SIN	3	0
3	G	221	SIN	3	0
3	D	225	SIN	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	219	SIN	1	0
3	G	220	SIN	2	0
4	D	227	MLI	2	0
3	C	227	SIN	1	0
3	C	228	SIN	3	0
3	C	222	SIN	12	0
3	E	222	SIN	7	0
3	B	220	SIN	1	0
3	C	225	SIN	2	0
2	F	219	TLA	1	0
3	E	221	SIN	3	0
4	B	225	MLI	7	0
3	A	220	SIN	2	0
3	C	224	SIN	1	0
3	F	223	SIN	3	0
3	B	222	SIN	8	0
3	E	218	SIN	4	0
4	C	232	MLI	1	0
4	D	228	MLI	2	0
4	E	223	MLI	7	0
6	B	218	FLC	5	0
3	D	221	SIN	1	0
3	A	219	SIN	15	0
2	H	218	TLA	4	0
3	C	221	SIN	1	0
3	A	221	SIN	10	0
2	A	218	TLA	1	0
3	D	222	SIN	2	0
4	G	224	MLI	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/220 (96%)	-0.50	2 (0%) 84 82	20, 32, 52, 66	0
1	B	213/220 (96%)	-0.24	5 (2%) 60 58	23, 40, 61, 96	0
1	C	212/220 (96%)	-0.69	2 (0%) 84 82	17, 27, 46, 75	0
1	D	213/220 (96%)	-0.48	2 (0%) 84 82	18, 29, 46, 59	0
1	E	213/220 (96%)	-0.48	2 (0%) 84 82	21, 34, 55, 76	0
1	F	213/220 (96%)	-0.30	4 (1%) 66 64	21, 34, 58, 86	0
1	G	212/220 (96%)	-0.32	5 (2%) 59 57	25, 39, 59, 88	0
1	H	214/220 (97%)	-0.26	3 (1%) 75 73	27, 42, 65, 74	0
All	All	1703/1760 (96%)	-0.41	25 (1%) 73 72	17, 34, 57, 96	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	0	ALA	7.4
1	F	-1	ASN	5.3
1	B	0	ALA	5.2
1	B	-1	ASN	4.7
1	E	0	ALA	4.2
1	C	0	ALA	4.1
1	B	180	GLU	3.5
1	H	-1	ASN	3.4
1	H	-2	SER	3.3
1	E	-1	ASN	3.3
1	A	0	ALA	3.2
1	F	147	VAL	3.0
1	F	0	ALA	2.9
1	B	123	PHE	2.8
1	G	147	VAL	2.7
1	A	-1	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	180[A]	GLU	2.3
1	D	0	ALA	2.3
1	H	130	VAL	2.3
1	D	-1	ASN	2.2
1	G	148	GLY	2.2
1	G	145	LEU	2.2
1	B	130	VAL	2.1
1	F	133	LYS	2.1
1	G	180	GLU	2.1

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. 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	B-factors(Å ²)	Q<0.9
3	SIN	H	222	8/8	0.63	0.66	41,51,54,56	8
3	SIN	C	223	8/8	0.65	0.39	78,92,98,98	0
3	SIN	H	221	8/8	0.66	0.26	92,94,95,96	0
3	SIN	G	219	8/8	0.67	0.25	76,82,87,89	0
3	SIN	E	220	8/8	0.68	0.24	69,80,88,89	0
3	SIN	C	228	8/8	0.69	0.76	28,32,36,38	8
2	TLA	C	219	10/10	0.69	0.22	44,50,52,52	10
3	SIN	F	222	8/8	0.71	0.30	49,56,58,58	8
3	SIN	G	222	8/8	0.73	0.26	32,49,57,58	8
4	MLI	C	232	7/7	0.74	0.41	13,26,34,38	7
3	SIN	F	221	8/8	0.75	0.28	93,95,99,100	0
3	SIN	B	222	8/8	0.75	0.39	18,24,30,31	8
3	SIN	A	219	8/8	0.75	0.38	29,36,41,43	8
3	SIN	C	224	8/8	0.75	0.37	14,27,37,38	8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SIN	F	223	8/8	0.76	0.32	81,90,93,93	0
3	SIN	B	221	8/8	0.76	0.21	63,72,80,80	0
4	MLI	B	225	7/7	0.76	0.44	20,27,36,39	7
3	SIN	A	224	8/8	0.76	0.31	45,49,54,55	8
3	SIN	E	222	8/8	0.77	0.31	31,32,41,42	8
4	MLI	A	225	7/7	0.77	0.43	21,26,33,33	7
6	FLC	B	218	13/13	0.77	0.41	39,49,53,55	13
3	SIN	A	223	8/8	0.78	0.38	42,47,55,59	8
3	SIN	C	227	8/8	0.78	0.36	35,41,44,44	8
4	MLI	D	226	7/7	0.79	0.39	26,31,38,42	7
3	SIN	E	219	8/8	0.79	0.20	75,78,83,83	0
2	TLA	A	218	10/10	0.79	0.32	47,56,58,63	10
3	SIN	D	221	8/8	0.80	0.33	20,27,39,47	8
3	SIN	C	221	8/8	0.80	0.40	41,44,46,48	8
4	MLI	G	224	7/7	0.80	0.19	56,59,61,62	7
4	MLI	D	227	7/7	0.81	0.36	31,32,41,43	7
3	SIN	D	220	8/8	0.81	0.18	58,71,74,75	0
3	SIN	E	221	8/8	0.81	0.23	82,88,91,93	0
4	MLI	D	228	7/7	0.81	0.31	29,37,43,47	7
4	MLI	B	224	7/7	0.81	0.21	60,61,64,65	7
3	SIN	G	221	8/8	0.82	0.27	75,79,88,89	0
3	SIN	A	220	8/8	0.82	0.31	76,83,91,92	0
3	SIN	H	223	8/8	0.82	0.21	52,55,56,57	8
6	FLC	F	218	13/13	0.83	0.38	9,26,30,36	13
7	NA	E	226	1/1	0.84	0.20	55,55,55,55	0
4	MLI	C	230	7/7	0.84	0.21	49,51,53,55	7
3	SIN	H	220	8/8	0.84	0.21	63,70,73,74	8
4	MLI	F	224	7/7	0.84	0.19	47,50,51,53	7
3	SIN	A	221	8/8	0.86	0.53	16,23,36,47	8
3	SIN	C	225	8/8	0.86	0.35	16,25,36,39	8
2	TLA	C	218	10/10	0.87	0.46	112,115,116,116	0
3	SIN	C	226	8/8	0.87	0.27	2,12,24,29	8
3	SIN	G	220	8/8	0.87	0.30	19,26,27,33	8
3	SIN	G	218	8/8	0.87	0.36	86,89,92,93	0
3	SIN	C	222	8/8	0.87	0.30	3,10,22,43	8
3	SIN	B	220	8/8	0.87	0.18	47,52,55,56	8
4	MLI	C	231	7/7	0.88	0.55	22,29,41,43	7
3	SIN	D	222	8/8	0.88	0.17	43,53,61,62	8
3	SIN	C	220	8/8	0.88	0.20	40,61,76,76	0
3	SIN	D	223	8/8	0.88	0.27	6,11,25,26	8
8	ACT	C	233	4/4	0.89	0.21	61,64,64,65	0
3	SIN	H	219	8/8	0.89	0.33	15,26,33,34	8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MLI	A	228	7/7	0.89	0.19	74,82,87,89	0
3	SIN	D	224	8/8	0.89	0.32	10,22,30,42	8
4	MLI	A	226	7/7	0.89	0.23	41,48,63,65	0
4	MLI	E	223	7/7	0.89	0.31	14,17,31,37	7
3	SIN	F	220	8/8	0.89	0.19	48,65,76,78	0
3	SIN	D	225	8/8	0.90	0.25	61,62,79,83	0
7	NA	C	238	1/1	0.90	0.14	59,59,59,59	0
3	SIN	A	222	8/8	0.90	0.41	23,61,73,82	0
2	TLA	H	218	10/10	0.92	0.21	40,57,64,74	0
3	SIN	E	218	8/8	0.93	0.20	33,48,62,63	0
8	ACT	D	229	4/4	0.93	0.23	51,52,53,54	0
3	SIN	D	219	8/8	0.94	0.16	44,55,64,72	0
5	CL	D	230	1/1	0.95	0.24	70,70,70,70	0
7	NA	B	227	1/1	0.95	0.10	56,56,56,56	0
4	MLI	H	224	7/7	0.95	0.32	32,37,47,50	7
4	MLI	G	223	7/7	0.95	0.52	14,17,25,25	7
2	TLA	B	219	10/10	0.95	0.16	41,52,65,70	0
5	CL	E	224	1/1	0.95	0.31	80,80,80,80	0
8	ACT	G	225	4/4	0.96	0.14	69,69,69,69	0
5	CL	G	226	1/1	0.96	0.35	59,59,59,59	0
5	CL	D	231	1/1	0.96	0.17	30,30,30,30	1
4	MLI	C	229	7/7	0.96	0.17	35,37,47,50	0
4	MLI	B	223	7/7	0.96	0.11	33,36,47,50	0
4	MLI	A	227	7/7	0.96	0.58	10,16,18,18	7
5	CL	B	226	1/1	0.96	0.05	68,68,68,68	0
2	TLA	D	218	10/10	0.96	0.12	24,31,37,46	0
7	NA	H	225	1/1	0.97	0.12	49,49,49,49	0
5	CL	F	225	1/1	0.98	0.24	80,80,80,80	0
2	TLA	F	219	10/10	0.98	0.13	29,37,52,54	0
5	CL	C	235	1/1	0.98	0.17	28,28,28,28	1
5	CL	E	225	1/1	0.98	0.30	66,66,66,66	0
5	CL	C	234	1/1	0.98	0.04	53,53,53,53	0
5	CL	C	236	1/1	0.98	0.26	67,67,67,67	0
5	CL	C	237	1/1	0.99	0.28	68,68,68,68	0
5	CL	A	229	1/1	0.99	0.10	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.