



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 02:52 PM EST

PDB ID : 5K4Y
Title : Three-dimensional structure of L-threonine 3-dehydrogenase from Trypanosoma brucei refined to 1.77 angstroms
Authors : Adjogatse, E.A.; Erskine, P.T.; Cooper, J.B.
Deposited on : 2016-05-22
Resolution : 1.77 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-20030736
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-20030736

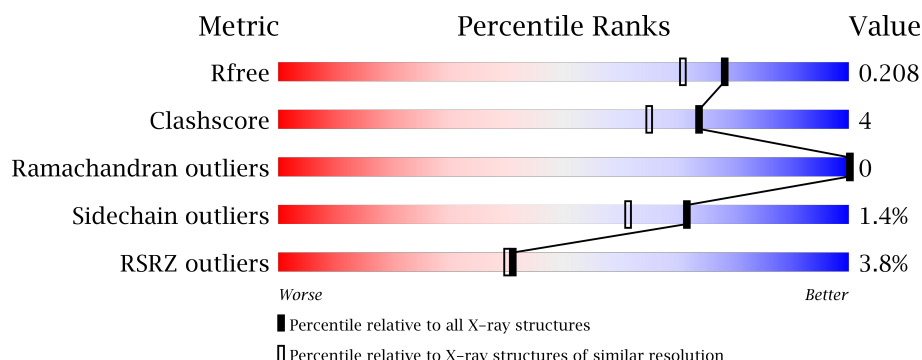
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	7172 (1.80-1.76)
Clashscore	112137	8247 (1.80-1.76)
Ramachandran outliers	110173	8154 (1.80-1.76)
Sidechain outliers	110143	8153 (1.80-1.76)
RSRZ outliers	101464	7262 (1.80-1.76)

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	320	<div> <div>3%</div> <div>91%</div> <div>9%</div> </div>
1	B	320	<div> <div>4%</div> <div>93%</div> <div>7%</div> </div>
1	C	320	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
1	D	320	<div> <div>4%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	E	320	<div> <div>4%</div> <div>90%</div> <div>9%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	320	

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
3	ACT	C	3402	-	-	X	-
3	ACT	F	6403	-	-	X	-
4	CL	D	4404	-	-	-	X
5	NA	E	5404	-	-	-	X
6	GOL	F	6402	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16948 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 L-threonine 3-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	4	0
			2521	1608	417	477	19			
1	B	320	Total	C	N	O	S	0	3	0
			2518	1606	418	474	20			
1	C	320	Total	C	N	O	S	0	4	0
			2525	1611	420	475	19			
1	D	320	Total	C	N	O	S	0	12	0
			2564	1636	426	482	20			
1	E	319	Total	C	N	O	S	0	5	0
			2524	1611	420	474	19			
1	F	320	Total	C	N	O	S	0	8	0
			2540	1623	421	475	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	MET	-	initiating methionine	UNP Q7YW97
B	2002	MET	-	initiating methionine	UNP Q7YW97
C	3002	MET	-	initiating methionine	UNP Q7YW97
D	4002	MET	-	initiating methionine	UNP Q7YW97
E	5002	MET	-	initiating methionine	UNP Q7YW97
F	6002	MET	-	initiating methionine	UNP Q7YW97

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	B	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	C	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	D	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	E	1	Total 44	C 21	N 7	O 14	P 2	0	0
2	F	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

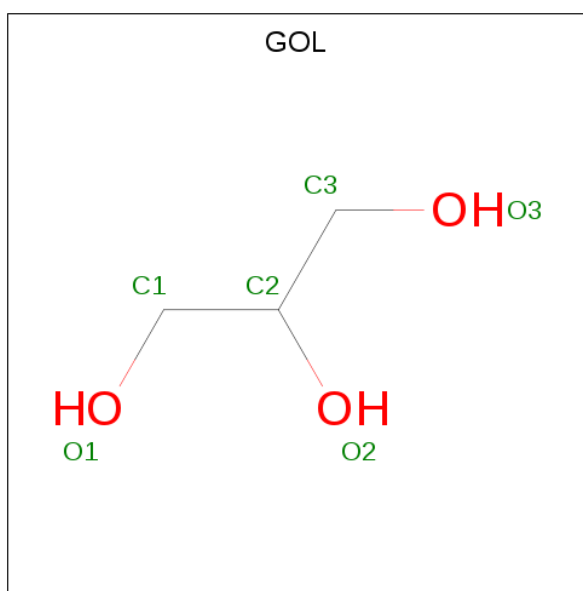
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	249	Total	O	0	0
			249	249		
7	B	240	Total	O	0	0
			240	240		

Continued on next page...

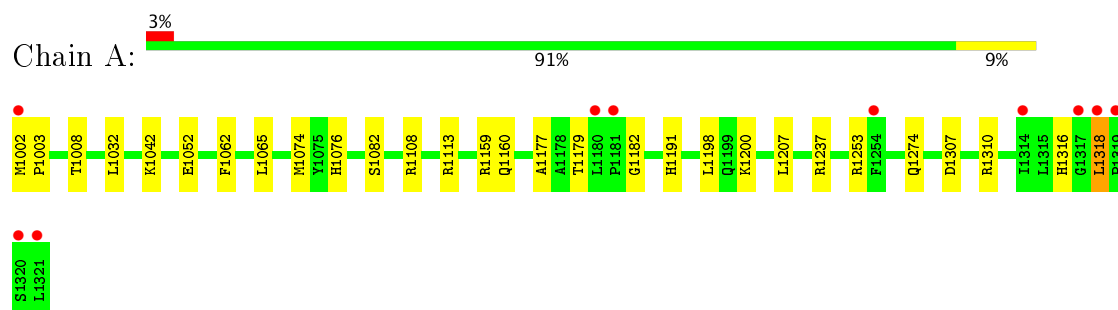
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	270	Total 270	O 270	0	0
7	D	231	Total 231	O 231	0	0
7	E	219	Total 219	O 219	0	0
7	F	239	Total 239	O 239	0	0

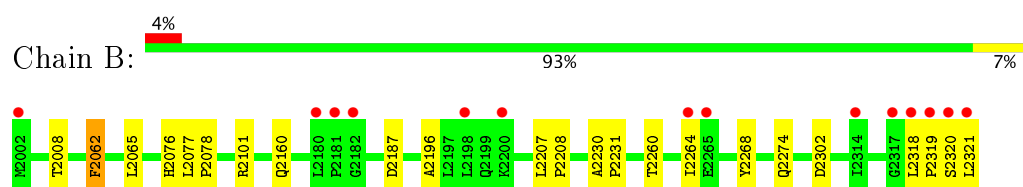
3 Residue-property plots [i](#)

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.

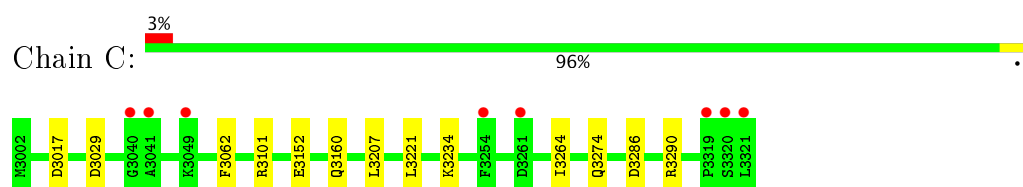
- Molecule 1: L-threonine 3-dehydrogenase



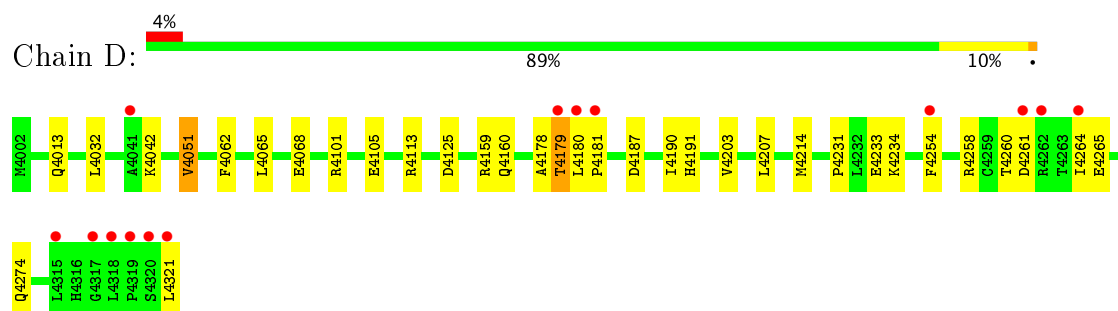
- Molecule 1: L-threonine 3-dehydrogenase



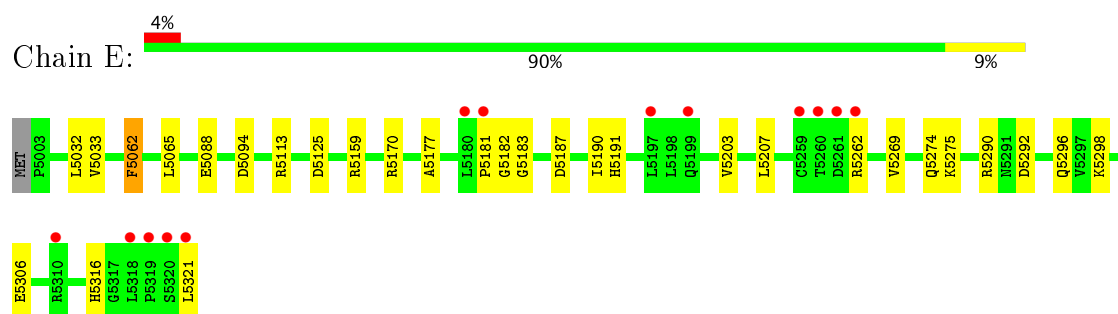
- Molecule 1: L-threonine 3-dehydrogenase



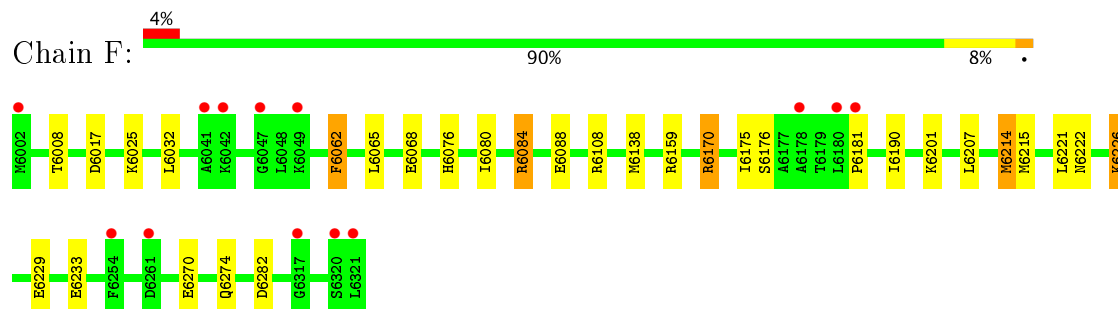
- Molecule 1: L-threonine 3-dehydrogenase



- Molecule 1: L-threonine 3-dehydrogenase



- Molecule 1: L-threonine 3-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.45Å 278.63Å 56.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.60 – 1.77 39.03 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-1.77) 99.8 (39.03-1.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.161 , 0.201 0.172 , 0.208	Depositor DCC
R_{free} test set	10231 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.53 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8140e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, NA, NAD, CL

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	0.98	1/2589 (0.0%)	1.07	6/3512 (0.2%)
1	B	0.96	0/2580	1.00	4/3499 (0.1%)
1	C	1.02	1/2590 (0.0%)	0.97	0/3514
1	D	1.01	2/2639 (0.1%)	1.01	9/3579 (0.3%)
1	E	0.94	0/2592	1.01	10/3513 (0.3%)
1	F	0.99	0/2620	1.05	12/3550 (0.3%)
All	All	0.98	4/15610 (0.0%)	1.02	41/21167 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4233	GLU	CD-OE2	6.35	1.32	1.25
1	D	4214	MET	SD-CE	-6.35	1.42	1.77
1	A	1237	ARG	CD-NE	-6.27	1.35	1.46
1	C	3152	GLU	CD-OE1	5.17	1.31	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1237	ARG	NE-CZ-NH1	18.32	129.46	120.30
1	A	1237	ARG	NE-CZ-NH2	-16.35	112.12	120.30
1	F	6084	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	E	5094	ASP	CB-CG-OD1	9.54	126.88	118.30
1	A	1108	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	F	6214	MET	CG-SD-CE	8.28	113.45	100.20
1	E	5113	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	F	6084	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	2062	PHE	CB-CG-CD1	7.12	125.78	120.80
1	E	5159	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	4113	ARG	NE-CZ-NH1	-6.99	116.80	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2062	PHE	CB-CG-CD2	-6.89	115.98	120.80
1	E	5094	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	E	5125	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	4101	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	D	4125	ASP	CB-CG-OD1	6.64	124.28	118.30
1	F	6159	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	B	2302	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	1253	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	4101	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	E	5159	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	D	4159	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	F	6282	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1253	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	F	6062	PHE	CB-CG-CD1	5.81	124.86	120.80
1	E	5170	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	F	6170	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	4113	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	1113	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	E	5290	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	4125	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	E	5062	PHE	CB-CG-CD1	5.36	124.55	120.80
1	F	6170	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	E	5292	ASP	CB-CG-OD1	5.29	123.06	118.30
1	F	6226[A]	LYS	CB-CA-C	-5.26	99.87	110.40
1	F	6226[B]	LYS	CB-CA-C	-5.26	99.87	110.40
1	D	4051	VAL	CG1-CB-CG2	5.17	119.18	110.90
1	D	4190	ILE	CB-CA-C	5.09	121.78	111.60
1	F	6215	MET	CG-SD-CE	5.08	108.33	100.20
1	B	2187	ASP	CB-CG-OD1	5.07	122.86	118.30
1	F	6108	ARG	NE-CZ-NH2	5.05	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2521	0	2535	19	0
1	B	2518	0	2533	15	0
1	C	2525	0	2545	10	0
1	D	2564	0	2592	24	0
1	E	2524	0	2549	14	0
1	F	2540	0	2579	29	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	0	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
3	C	4	0	3	3	0
3	D	4	0	3	0	0
3	E	4	0	3	0	0
3	F	4	0	3	3	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	F	6	0	8	2	0
7	A	249	0	0	8	0
7	B	240	0	0	5	0
7	C	270	0	0	10	0
7	D	231	0	0	5	0
7	E	219	0	0	7	0
7	F	239	0	0	8	0
All	All	16948	0	15515	117	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 4.

All (117) 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:E:5191:HIS:NE2	7:E:5501:HOH:O	1.81	1.13
1:A:1160[A]:GLN:HG3	7:A:1590:HOH:O	1.61	0.99
1:D:4187:ASP:HB2	7:D:4538:HOH:O	1.66	0.94
1:A:1160[A]:GLN:OE1	7:A:1501:HOH:O	1.87	0.91
1:D:4187:ASP:CB	7:D:4538:HOH:O	2.20	0.89
1:C:3264:ILE:HG23	7:C:3567:HOH:O	1.73	0.86
1:C:3286:ASP:OD1	1:C:3290[B]:ARG:NH1	2.11	0.83
1:F:6138[B]:MET:HE3	1:F:6170:ARG:NH2	1.93	0.82
1:B:2160[A]:GLN:OE1	7:B:2501:HOH:O	1.99	0.80
3:C:3402:ACT:H2	7:C:3534:HOH:O	1.81	0.79
1:E:5187:ASP:HB2	7:E:5516:HOH:O	1.82	0.78
1:D:4032:LEU:HD21	1:D:4065:LEU:HD11	1.66	0.78
1:F:6226[B]:LYS:NZ	7:F:6501:HOH:O	1.62	0.77
1:D:4180[A]:LEU:HD23	1:D:4181[A]:PRO:N	2.01	0.76
1:E:5183:GLY:HA2	7:E:5504:HOH:O	1.85	0.76
1:F:6084:ARG:HD2	1:F:6088:GLU:OE1	1.86	0.76
3:F:6403:ACT:H2	7:F:6503:HOH:O	1.89	0.72
1:D:4105:GLU:OE2	7:D:4502:HOH:O	2.10	0.70
1:B:2101:ARG:HG3	7:B:2502:HOH:O	1.90	0.70
1:F:6222:ASN:ND2	1:F:6226[B]:LYS:HD3	2.08	0.68
1:D:4187:ASP:OD2	7:D:4503:HOH:O	2.12	0.68
1:E:5032:LEU:HD21	1:E:5065:LEU:HD11	1.76	0.68
3:C:3402:ACT:H1	7:C:3642:HOH:O	1.93	0.68
1:D:4013:GLN:HG3	1:D:4179[A]:THR:HG21	1.75	0.67
1:F:6226[B]:LYS:CE	7:F:6501:HOH:O	2.27	0.67
3:F:6403:ACT:H1	7:F:6555:HOH:O	1.95	0.67
1:A:1082[A]:SER:OG	4:A:1403:CL:CL	2.50	0.66
1:A:1160[A]:GLN:CD	7:A:1501:HOH:O	2.31	0.65
1:E:5191:HIS:CE1	7:E:5501:HOH:O	2.38	0.64
1:F:6068:GLU:HG3	7:F:6597:HOH:O	1.98	0.63
1:F:6222:ASN:O	1:F:6226[B]:LYS:HB2	1.98	0.63
1:A:1032:LEU:HD21	1:A:1065:LEU:HD11	1.79	0.63
1:F:6222:ASN:HD21	1:F:6226[B]:LYS:NZ	1.97	0.62
1:F:6175:ILE:HD11	1:F:6214:MET:CE	2.30	0.61
1:A:1159:ARG:NH2	7:A:1505:HOH:O	2.33	0.60
1:A:1177:ALA:O	1:A:1316:HIS:HE1	1.85	0.60
1:B:2196:ALA:CA	1:B:2264:ILE:HD12	2.31	0.59
1:C:3290[B]:ARG:NH1	7:C:3504:HOH:O	2.35	0.59
1:B:2207:LEU:H	1:B:2274:GLN:NE2	2.01	0.59
1:F:6222:ASN:CG	1:F:6226[B]:LYS:HD3	2.22	0.58
1:C:3160:GLN:CD	7:C:3502:HOH:O	2.41	0.58
1:D:4207:LEU:H	1:D:4274:GLN:NE2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4181[A]:PRO:HB2	1:D:4191:HIS:CE1	2.39	0.58
1:C:3207:LEU:H	1:C:3274:GLN:NE2	2.02	0.56
1:F:6138[B]:MET:CE	1:F:6170:ARG:NH2	2.66	0.56
1:C:3160:GLN:HG2	7:C:3736:HOH:O	2.06	0.55
1:D:4180[A]:LEU:CD2	1:D:4181[A]:PRO:O	2.55	0.55
1:F:6138[B]:MET:CE	7:F:6633:HOH:O	2.54	0.55
1:F:6138[B]:MET:HE3	7:F:6633:HOH:O	2.07	0.54
1:B:2196:ALA:HA	1:B:2264:ILE:HD12	1.88	0.54
1:F:6032:LEU:HD21	1:F:6065:LEU:HD11	1.90	0.54
1:A:1032:LEU:HD11	1:A:1052:GLU:HG3	1.90	0.54
1:B:2160[B]:GLN:NE2	7:B:2501:HOH:O	2.38	0.54
1:F:6176:SER:HB2	6:F:6402:GOL:H31	1.90	0.54
1:D:4178[A]:ALA:O	1:D:4179[A]:THR:HG23	2.08	0.54
1:B:2101:ARG:CG	7:B:2502:HOH:O	2.50	0.53
1:D:4254:PHE:HD1	1:D:4258:ARG:NH1	2.07	0.52
1:F:6207:LEU:H	1:F:6274:GLN:NE2	2.08	0.51
1:D:4180[A]:LEU:HD23	1:D:4181[A]:PRO:CD	2.41	0.51
1:D:4180[A]:LEU:HD23	1:D:4180[A]:LEU:C	2.31	0.51
1:B:2260:THR:HG22	1:B:2321:LEU:HD21	1.93	0.50
1:C:3017:ASP:HB3	1:C:3221:LEU:HD11	1.92	0.50
1:D:4254:PHE:CD1	1:D:4258:ARG:NH1	2.79	0.50
1:A:1207:LEU:H	1:A:1274:GLN:NE2	2.10	0.50
1:B:2065:LEU:HD23	1:B:2065:LEU:C	2.32	0.50
3:F:6403:ACT:CH3	7:F:6555:HOH:O	2.58	0.50
1:F:6222:ASN:ND2	1:F:6226[B]:LYS:CD	2.75	0.50
1:F:6025:LYS:HE2	1:F:6229:GLU:OE2	2.11	0.50
1:A:1307:ASP:OD1	1:A:1310:ARG:NH2	2.41	0.49
1:E:5181:PRO:C	7:E:5501:HOH:O	2.51	0.49
3:C:3402:ACT:CH3	7:C:3642:HOH:O	2.56	0.49
1:B:2160[A]:GLN:CD	7:B:2501:HOH:O	2.47	0.49
1:D:4013:GLN:HG3	1:D:4179[A]:THR:CG2	2.41	0.49
1:A:1179:THR:HG22	7:A:1530:HOH:O	2.13	0.49
1:A:1182:GLY:O	1:A:1191:HIS:HE1	1.95	0.49
1:A:1002:MET:HB2	1:A:1003:PRO:HD2	1.94	0.48
1:E:5088:GLU:OE2	7:E:5502:HOH:O	2.20	0.47
1:A:1191:HIS:HD2	7:A:1729:HOH:O	1.98	0.47
1:C:3160:GLN:OE1	7:C:3502:HOH:O	2.20	0.47
1:E:5207:LEU:H	1:E:5274:GLN:NE2	2.12	0.47
1:A:1160[A]:GLN:CG	7:A:1590:HOH:O	2.40	0.46
1:E:5203:VAL:HG13	1:E:5269:VAL:HG13	1.97	0.46
1:D:4180[A]:LEU:C	1:D:4180[A]:LEU:CD2	2.84	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5177:ALA:O	1:E:5316:HIS:HE1	1.98	0.45
1:B:2008:THR:OG1	1:B:2076:HIS:HA	2.17	0.45
1:F:6008:THR:OG1	1:F:6076:HIS:HA	2.17	0.45
1:D:4260:THR:HG22	1:D:4321:LEU:HD21	1.98	0.45
1:F:6222:ASN:ND2	1:F:6226[B]:LYS:CE	2.80	0.45
1:C:3029:ASP:OD1	7:C:3503:HOH:O	2.21	0.44
1:F:6181:PRO:HA	1:F:6190:ILE:HD11	2.00	0.44
1:A:1160[A]:GLN:HG2	7:A:1733:HOH:O	2.16	0.44
1:F:6233:GLU:CD	1:F:6233:GLU:H	2.21	0.44
1:F:6270:GLU:HG3	1:F:6274:GLN:HB3	1.99	0.43
1:D:4231:PRO:HD2	1:D:4234:LYS:HD3	2.01	0.43
1:E:5182:GLY:C	7:E:5504:HOH:O	2.57	0.43
1:F:6017:ASP:HB3	1:F:6221:LEU:HD11	2.00	0.43
1:F:6222:ASN:HD21	1:F:6226[B]:LYS:CE	2.32	0.42
1:A:1198:LEU:HG	1:A:1318:LEU:HD13	2.01	0.42
1:C:3101:ARG:HG3	7:C:3514:HOH:O	2.20	0.42
1:E:5181:PRO:HB3	1:E:5190:ILE:HG22	2.00	0.42
1:F:6176:SER:HB2	6:F:6402:GOL:C3	2.48	0.42
1:D:4181[A]:PRO:CB	1:D:4191:HIS:CE1	3.03	0.42
1:F:6222:ASN:HD21	1:F:6226[B]:LYS:HZ3	1.67	0.41
1:E:5306:GLU:HA	1:E:5306:GLU:OE1	2.19	0.41
1:F:6080:ILE:HG23	1:F:6084:ARG:HG2	2.02	0.41
1:B:2077:LEU:N	1:B:2078:PRO:CD	2.84	0.41
1:B:2230:ALA:HA	1:B:2231:PRO:HD3	1.97	0.41
1:B:2208:PRO:HB3	1:B:2268:TYR:CZ	2.55	0.41
1:A:1002:MET:HB2	1:A:1003:PRO:CD	2.51	0.41
1:A:1008:THR:OG1	1:A:1076:HIS:HA	2.21	0.41
1:D:4187:ASP:HB3	7:D:4538:HOH:O	2.03	0.40
1:F:6175:ILE:HD11	1:F:6214:MET:HE3	2.04	0.40
1:D:4203:VAL:HG23	1:D:4203:VAL:O	2.21	0.40
1:E:5296:GLN:HE21	1:E:5298:LYS:NZ	2.19	0.40
1:B:2318:LEU:HB3	1:B:2319:PRO:CD	2.52	0.40
1:D:4180[A]:LEU:HD22	1:D:4181[A]:PRO:O	2.20	0.40
1:D:4264:ILE:HG12	1:D:4265:GLU:N	2.37	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	322/320 (101%)	316 (98%)	6 (2%)	0	100	100
1	B	321/320 (100%)	317 (99%)	4 (1%)	0	100	100
1	C	322/320 (101%)	315 (98%)	7 (2%)	0	100	100
1	D	330/320 (103%)	321 (97%)	9 (3%)	0	100	100
1	E	322/320 (101%)	317 (98%)	5 (2%)	0	100	100
1	F	326/320 (102%)	321 (98%)	5 (2%)	0	100	100
All	All	1943/1920 (101%)	1907 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/277 (101%)	276 (98%)	5 (2%)	64	50
1	B	280/277 (101%)	278 (99%)	2 (1%)	87	82
1	C	281/277 (101%)	279 (99%)	2 (1%)	87	82
1	D	286/277 (103%)	277 (97%)	9 (3%)	45	26
1	E	281/277 (101%)	276 (98%)	5 (2%)	64	50
1	F	285/277 (103%)	283 (99%)	2 (1%)	87	82
All	All	1694/1662 (102%)	1669 (98%)	25 (2%)	71	58

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1042	LYS
1	A	1062	PHE
1	A	1074	MET
1	A	1200	LYS
1	A	1318	LEU
1	B	2062	PHE
1	B	2320	SER
1	C	3062	PHE
1	C	3234	LYS
1	D	4042	LYS
1	D	4051	VAL
1	D	4062	PHE
1	D	4068	GLU
1	D	4160[A]	GLN
1	D	4160[B]	GLN
1	D	4179[A]	THR
1	D	4179[B]	THR
1	D	4261	ASP
1	E	5033	VAL
1	E	5062	PHE
1	E	5262	ARG
1	E	5275	LYS
1	E	5321	LEU
1	F	6062	PHE
1	F	6201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1191	HIS
1	A	1274	GLN
1	A	1278	ASN
1	A	1316	HIS
1	B	2274	GLN
1	B	2278	ASN
1	C	3222	ASN
1	C	3274	GLN
1	D	4191	HIS
1	D	4274	GLN
1	D	4278	ASN
1	E	5274	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	5278	ASN
1	E	5296	GLN
1	E	5311	GLN
1	E	5316	HIS
1	F	6222	ASN
1	F	6274	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	NAD	A	1401	-	41,48,48	1.31	2 (4%)	43,73,73	1.84	5 (11%)
3	ACT	A	1402	-	1,3,3	2.36	1 (100%)	0,3,3	0.00	-
2	NAD	B	2401	-	41,48,48	1.29	4 (9%)	43,73,73	1.76	8 (18%)
3	ACT	B	2402	-	1,3,3	0.17	0	0,3,3	0.00	-
2	NAD	C	3401	-	41,48,48	1.58	8 (19%)	43,73,73	2.28	8 (18%)
3	ACT	C	3402	-	1,3,3	7.83	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	D	4401	-	41,48,48	1.46	6 (14%)	43,73,73	1.38	4 (9%)
3	ACT	D	4402	-	1,3,3	1.82	0	0,3,3	0.00	-
2	NAD	E	5401	-	41,48,48	1.47	9 (21%)	43,73,73	1.79	9 (20%)
3	ACT	E	5402	-	1,3,3	3.13	1 (100%)	0,3,3	0.00	-
2	NAD	F	6401	-	41,48,48	1.35	3 (7%)	43,73,73	1.68	6 (13%)
6	GOL	F	6402	-	5,5,5	0.67	0	5,5,5	1.98	2 (40%)
3	ACT	F	6403	-	1,3,3	4.85	1 (100%)	0,3,3	0.00	-

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	NAD	A	1401	-	-	0/22/62/62	0/5/5/5
3	ACT	A	1402	-	-	0/0/0/0	0/0/0/0
2	NAD	B	2401	-	-	0/22/62/62	0/5/5/5
3	ACT	B	2402	-	-	0/0/0/0	0/0/0/0
2	NAD	C	3401	-	-	0/22/62/62	0/5/5/5
3	ACT	C	3402	-	-	0/0/0/0	0/0/0/0
2	NAD	D	4401	-	-	0/22/62/62	0/5/5/5
3	ACT	D	4402	-	-	0/0/0/0	0/0/0/0
2	NAD	E	5401	-	-	0/22/62/62	0/5/5/5
3	ACT	E	5402	-	-	0/0/0/0	0/0/0/0
2	NAD	F	6401	-	-	0/22/62/62	0/5/5/5
6	GOL	F	6402	-	-	0/4/4/4	0/0/0/0
3	ACT	F	6403	-	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3402	ACT	CH3-C	-7.83	1.38	1.48
3	F	6403	ACT	CH3-C	-4.85	1.42	1.48
2	C	3401	NAD	C2D-C1D	-3.15	1.48	1.53
2	D	4401	NAD	O4B-C1B	-2.89	1.37	1.41
2	D	4401	NAD	C8A-N7A	-2.52	1.30	1.34
2	C	3401	NAD	C5A-C4A	-2.05	1.35	1.40
2	B	2401	NAD	O4B-C1B	-2.01	1.38	1.41
2	E	5401	NAD	C2N-C3N	2.08	1.42	1.39
2	C	3401	NAD	O4B-C1B	2.11	1.44	1.41
2	E	5401	NAD	C7N-N7N	2.16	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5401	NAD	C6N-C5N	2.16	1.43	1.38
2	F	6401	NAD	O7N-C7N	2.18	1.28	1.24
2	E	5401	NAD	C6N-N1N	2.21	1.41	1.35
2	C	3401	NAD	O3B-C3B	2.23	1.48	1.43
2	E	5401	NAD	O2B-C2B	2.28	1.48	1.43
3	A	1402	ACT	CH3-C	2.36	1.51	1.48
2	E	5401	NAD	O4D-C4D	2.38	1.50	1.45
2	F	6401	NAD	C6N-N1N	2.47	1.41	1.35
2	E	5401	NAD	O3D-C3D	2.50	1.48	1.43
2	B	2401	NAD	C6N-N1N	2.51	1.41	1.35
2	D	4401	NAD	C6N-N1N	2.51	1.41	1.35
2	F	6401	NAD	C3N-C7N	2.53	1.54	1.50
2	C	3401	NAD	O2B-C2B	2.65	1.49	1.43
2	D	4401	NAD	O3D-C3D	2.71	1.49	1.43
2	E	5401	NAD	O4D-C1D	2.90	1.45	1.41
2	D	4401	NAD	O2B-C2B	3.07	1.50	1.43
3	E	5402	ACT	CH3-C	3.13	1.52	1.48
2	B	2401	NAD	O2B-C2B	3.31	1.50	1.43
2	E	5401	NAD	O7N-C7N	3.33	1.31	1.24
2	C	3401	NAD	C6N-N1N	3.52	1.44	1.35
2	D	4401	NAD	O7N-C7N	3.67	1.31	1.24
2	C	3401	NAD	O7N-C7N	3.80	1.32	1.24
2	B	2401	NAD	O7N-C7N	3.88	1.32	1.24
2	A	1401	NAD	O2B-C2B	4.17	1.52	1.43
2	C	3401	NAD	O4D-C1D	4.21	1.47	1.41
2	A	1401	NAD	O4D-C1D	4.41	1.47	1.41

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3401	NAD	N3A-C2A-N1A	-11.02	119.26	128.86
2	A	1401	NAD	N3A-C2A-N1A	-9.84	120.29	128.86
2	B	2401	NAD	N3A-C2A-N1A	-6.92	122.83	128.86
2	F	6401	NAD	N3A-C2A-N1A	-6.44	123.25	128.86
2	E	5401	NAD	N3A-C2A-N1A	-6.37	123.31	128.86
2	D	4401	NAD	N3A-C2A-N1A	-5.11	124.41	128.86
2	C	3401	NAD	C4B-O4B-C1B	-5.10	104.34	109.77
2	F	6401	NAD	C4B-O4B-C1B	-4.10	105.40	109.77
2	E	5401	NAD	O7N-C7N-C3N	-3.86	115.11	119.62
2	B	2401	NAD	C5N-C4N-C3N	-3.80	115.88	120.35
2	B	2401	NAD	O7N-C7N-C3N	-3.49	115.54	119.62
2	C	3401	NAD	C3N-C2N-N1N	-3.27	117.13	120.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5401	NAD	C4B-O4B-C1B	-2.89	106.69	109.77
2	A	1401	NAD	C5B-C4B-C3B	-2.64	105.24	115.29
2	E	5401	NAD	C4A-C5A-N7A	-2.47	107.03	109.41
2	E	5401	NAD	C3N-C2N-N1N	-2.46	117.95	120.43
2	D	4401	NAD	C5N-C6N-N1N	-2.24	116.96	120.40
2	E	5401	NAD	C4N-C3N-C7N	-2.22	115.18	121.07
2	D	4401	NAD	C5N-C4N-C3N	-2.21	117.75	120.35
2	B	2401	NAD	O4D-C4D-C5D	-2.15	102.14	109.40
2	F	6401	NAD	O3D-C3D-C2D	-2.14	104.99	111.83
2	C	3401	NAD	O3D-C3D-C2D	-2.12	105.04	111.83
2	C	3401	NAD	O4B-C4B-C5B	-2.07	102.41	109.40
2	A	1401	NAD	C5N-C6N-N1N	-2.06	117.23	120.40
2	E	5401	NAD	O4B-C4B-C5B	-2.02	102.59	109.40
2	B	2401	NAD	C5D-C4D-C3D	2.04	123.07	115.29
2	F	6401	NAD	O2B-C2B-C1B	2.07	118.09	111.61
2	F	6401	NAD	O4B-C4B-C3B	2.15	109.45	105.17
6	F	6402	GOL	O3-C3-C2	2.19	121.11	110.07
2	A	1401	NAD	O2N-PN-O1N	2.21	123.73	112.28
2	C	3401	NAD	C5N-C4N-C3N	2.29	123.04	120.35
2	B	2401	NAD	C3N-C7N-N7N	2.33	120.43	117.77
2	F	6401	NAD	C2N-C3N-C4N	2.37	120.96	118.26
2	C	3401	NAD	O2N-PN-O1N	2.46	125.02	112.28
2	C	3401	NAD	C4A-C5A-N7A	2.47	111.80	109.41
2	A	1401	NAD	C3N-C7N-N7N	2.49	120.62	117.77
2	E	5401	NAD	O7N-C7N-N7N	2.90	126.70	122.58
2	B	2401	NAD	C2N-C3N-C4N	2.93	121.60	118.26
6	F	6402	GOL	O2-C2-C3	3.05	123.24	108.84
2	B	2401	NAD	C6N-C5N-C4N	3.05	124.04	119.44
2	D	4401	NAD	C6N-C5N-C4N	3.35	124.50	119.44
2	E	5401	NAD	C2N-C3N-C4N	4.26	123.12	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3402	ACT	3	0
6	F	6402	GOL	2	0
3	F	6403	ACT	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	320/320 (100%)	-0.08	10 (3%)	49	48	7, 15, 35, 79	0
1	B	320/320 (100%)	-0.02	14 (4%)	35	34	7, 16, 43, 55	0
1	C	320/320 (100%)	-0.11	8 (2%)	58	57	7, 15, 34, 46	0
1	D	320/320 (100%)	-0.00	14 (4%)	35	34	7, 15, 40, 51	0
1	E	319/320 (99%)	0.03	13 (4%)	38	37	7, 17, 46, 72	0
1	F	320/320 (100%)	-0.06	13 (4%)	38	37	8, 16, 39, 56	0
All	All	1919/1920 (99%)	-0.04	72 (3%)	41	40	7, 16, 40, 79	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1321	LEU	10.9
1	E	5321	LEU	9.5
1	D	4321	LEU	5.9
1	F	6321	LEU	5.8
1	C	3041	ALA	5.6
1	B	2321	LEU	4.7
1	F	6041	ALA	4.6
1	A	1319	PRO	4.3
1	B	2180	LEU	4.3
1	F	6254	PHE	4.2
1	C	3321	LEU	4.0
1	E	5320	SER	3.8
1	E	5318	LEU	3.8
1	E	5319	PRO	3.5
1	F	6047	GLY	3.5
1	A	1318	LEU	3.5
1	D	4254	PHE	3.3
1	E	5180	LEU	3.3
1	D	4264	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	6042	LYS	3.2
1	D	4041	ALA	3.2
1	B	2318	LEU	3.1
1	B	2198	LEU	3.1
1	C	3320	SER	3.0
1	D	4261	ASP	3.0
1	F	6180	LEU	2.9
1	D	4179[A]	THR	2.9
1	E	5181	PRO	2.8
1	F	6320	SER	2.8
1	C	3254	PHE	2.8
1	D	4318	LEU	2.8
1	E	5262	ARG	2.7
1	D	4319	PRO	2.7
1	F	6261	ASP	2.7
1	D	4317	GLY	2.6
1	D	4262	ARG	2.6
1	F	6317	GLY	2.6
1	A	1320	SER	2.6
1	F	6181	PRO	2.6
1	D	4180[A]	LEU	2.6
1	B	2320	SER	2.6
1	C	3049	LYS	2.5
1	B	2319	PRO	2.4
1	E	5261	ASP	2.4
1	F	6002	MET	2.4
1	C	3319	PRO	2.4
1	A	1002	MET	2.4
1	B	2314	ILE	2.3
1	A	1180	LEU	2.3
1	B	2265	GLU	2.3
1	D	4315	LEU	2.3
1	F	6178	ALA	2.3
1	C	3040	GLY	2.3
1	D	4181[A]	PRO	2.3
1	E	5260	THR	2.3
1	F	6049	LYS	2.3
1	B	2182	GLY	2.2
1	A	1254	PHE	2.2
1	C	3261	ASP	2.2
1	E	5310	ARG	2.2
1	B	2200	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	2002	MET	2.2
1	B	2317	GLY	2.1
1	B	2264	ILE	2.1
1	A	1181	PRO	2.1
1	B	2181	PRO	2.1
1	D	4320	SER	2.1
1	E	5197	LEU	2.1
1	A	1317	GLY	2.1
1	E	5259	CYS	2.1
1	A	1314	ILE	2.1
1	E	5199	GLN	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
6	GOL	F	6402	6/6	0.87	0.25	4.50	13,15,17,21	6
4	CL	D	4404	1/1	0.93	0.23	3.63	43,43,43,43	0
5	NA	E	5404	1/1	0.97	0.14	2.95	32,32,32,32	0
3	ACT	A	1402	4/4	0.96	0.10	0.88	14,16,16,19	0
3	ACT	C	3402	4/4	0.92	0.10	0.33	12,14,17,18	0
3	ACT	F	6403	4/4	0.94	0.09	0.06	13,15,17,20	0
3	ACT	E	5402	4/4	0.95	0.10	-0.03	15,16,19,19	0
3	ACT	D	4402	4/4	0.97	0.09	-0.19	14,15,16,19	0
4	CL	E	5403	1/1	0.94	0.09	-0.74	44,44,44,44	0
2	NAD	A	1401	44/44	0.98	0.07	-0.83	8,11,12,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAD	D	4401	44/44	0.98	0.07	-0.97	8,11,12,13	0
2	NAD	B	2401	44/44	0.98	0.07	-1.02	10,11,13,15	0
5	NA	D	4406	1/1	0.98	0.05	-1.12	31,31,31,31	0
2	NAD	E	5401	44/44	0.98	0.07	-1.18	9,12,14,15	0
2	NAD	F	6401	44/44	0.98	0.06	-1.20	9,12,15,16	0
5	NA	B	2404	1/1	0.97	0.09	-1.30	30,30,30,30	0
2	NAD	C	3401	44/44	0.98	0.07	-1.31	10,12,14,15	0
3	ACT	B	2402	4/4	0.98	0.07	-1.58	15,16,18,20	0
5	NA	F	6405	1/1	0.96	0.07	-1.75	27,27,27,27	0
4	CL	C	3403	1/1	0.99	0.04	-2.12	21,21,21,21	0
4	CL	D	4403	1/1	0.96	0.06	-2.27	32,32,32,32	0
4	CL	B	2403	1/1	0.95	0.09	-2.32	35,35,35,35	0
4	CL	A	1403	1/1	0.98	0.07	-2.45	34,34,34,34	0
5	NA	C	3404	1/1	0.99	0.03	-2.57	24,24,24,24	0
5	NA	D	4405	1/1	0.99	0.05	-3.20	29,29,29,29	0
4	CL	F	6404	1/1	0.98	0.05	-3.44	27,27,27,27	0
5	NA	A	1404	1/1	0.99	0.06	-3.75	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.