



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2017 – 01:31 AM EST

PDB ID : 3S55
Title : Crystal structure of a putative short-chain dehydrogenase/reductase from Mycobacterium abscessus bound to NAD
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2011-05-20
Resolution : 2.10 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

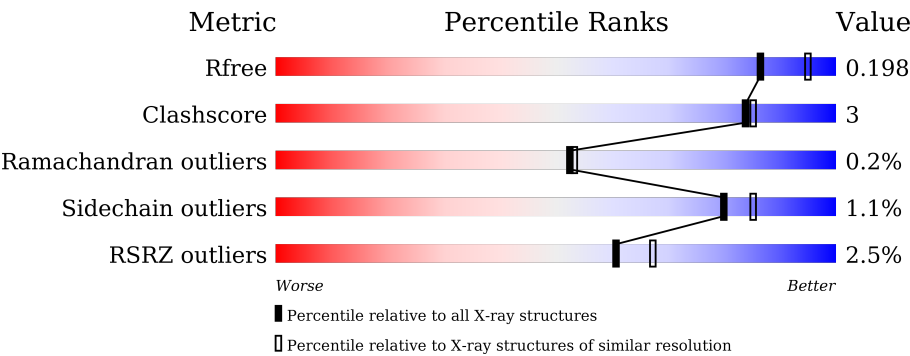
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	281	<div><div>3%</div><div>90%6%</div><div></div></div>
1	B	281	<div><div>2%</div><div>86%10%</div><div></div></div>
1	C	281	<div><div>2%</div><div>88%7%</div><div></div></div>
1	D	281	<div><div>4%</div><div>89%8%</div><div></div></div>
1	E	281	<div><div>2%</div><div>89%5%5%</div><div></div></div>
1	F	281	<div><div></div><div>90%8%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	281	<div><div></div><div>4%</div><div>89%</div><div>6%</div><div></div></div>
1	H	281	<div><div></div><div>2%</div><div>91%</div><div>6%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17342 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 Putative short-chain dehydrogenase/reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	2	0
			1957	1229	333	386	9			
1	B	270	Total	C	N	O	S	0	3	0
			1972	1240	334	389	9			
1	C	269	Total	C	N	O	S	0	2	0
			1955	1228	330	388	9			
1	D	275	Total	C	N	O	S	0	1	0
			1987	1249	335	393	10			
1	E	266	Total	C	N	O	S	0	2	0
			1922	1207	327	379	9			
1	F	275	Total	C	N	O	S	0	1	0
			2011	1260	343	398	10			
1	G	269	Total	C	N	O	S	0	3	0
			1955	1229	333	384	9			
1	H	271	Total	C	N	O	S	0	3	0
			1969	1242	332	385	10			

There are 32 discrepancies between the modelled and reference sequences:

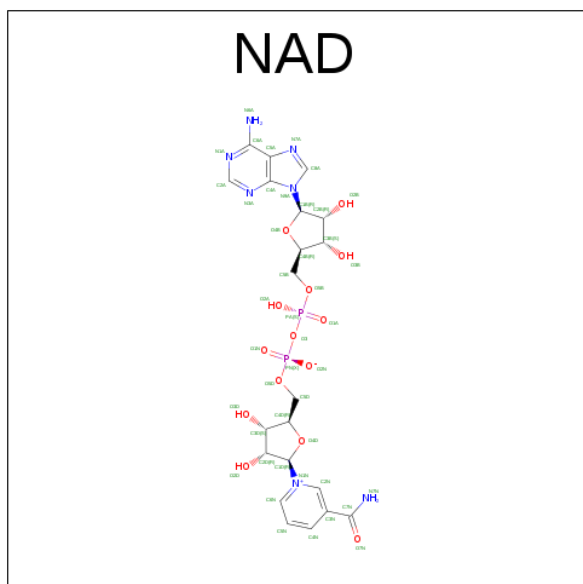
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
A	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
A	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
A	1	SER	-	EXPRESSION TAG	UNP B1MLR7
B	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
B	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
B	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
B	1	SER	-	EXPRESSION TAG	UNP B1MLR7
C	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
C	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
C	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
C	1	SER	-	EXPRESSION TAG	UNP B1MLR7
D	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
D	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
D	1	SER	-	EXPRESSION TAG	UNP B1MLR7
E	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
E	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
E	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
E	1	SER	-	EXPRESSION TAG	UNP B1MLR7
F	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
F	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
F	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
F	1	SER	-	EXPRESSION TAG	UNP B1MLR7
G	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
G	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
G	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
G	1	SER	-	EXPRESSION TAG	UNP B1MLR7
H	-2	GLY	-	EXPRESSION TAG	UNP B1MLR7
H	-1	PRO	-	EXPRESSION TAG	UNP B1MLR7
H	0	GLY	-	EXPRESSION TAG	UNP B1MLR7
H	1	SER	-	EXPRESSION TAG	UNP B1MLR7

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	B	2	Total	Ca	0	0
			2	2		
3	A	1	Total	Ca	0	0
			1	1		
3	F	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	153	Total	O	0	0
			153	153		
4	C	151	Total	O	0	0
			151	151		
4	D	145	Total	O	0	0
			145	145		

Continued on next page...


Continued from previous page...

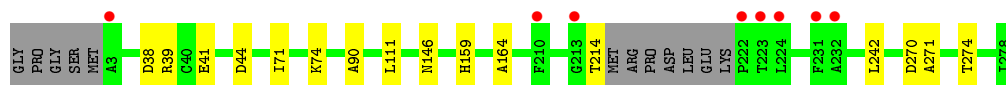
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	148	Total 148	O 148	0	0
4	F	185	Total 185	O 185	0	0
4	G	167	Total 167	O 167	0	0
4	H	160	Total 160	O 160	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

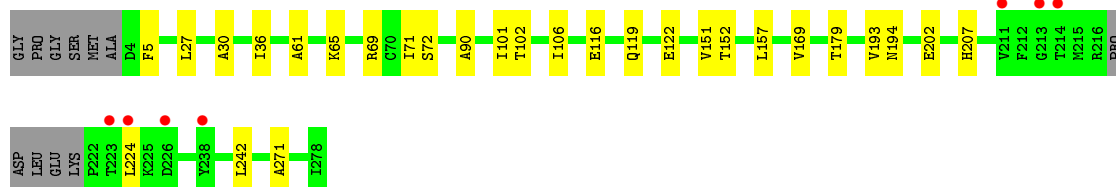
- Molecule 1: Putative short-chain dehydrogenase/reductase

Chain A: 




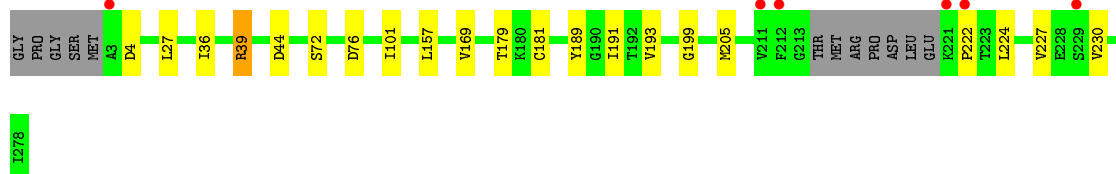
- Molecule 1: Putative short-chain dehydrogenase/reductase

Chain B: 




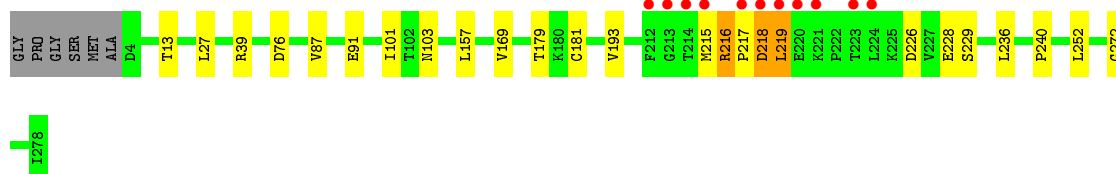
- Molecule 1: Putative short-chain dehydrogenase/reductase

Chain C: 

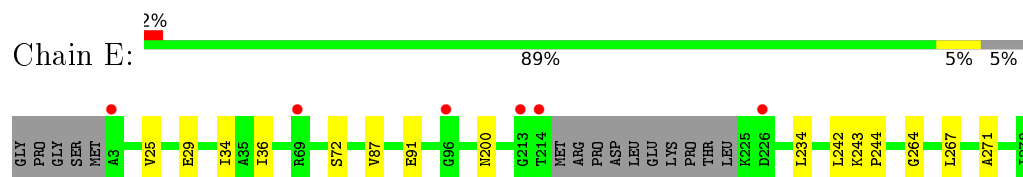


- Molecule 1: Putative short-chain dehydrogenase/reductase

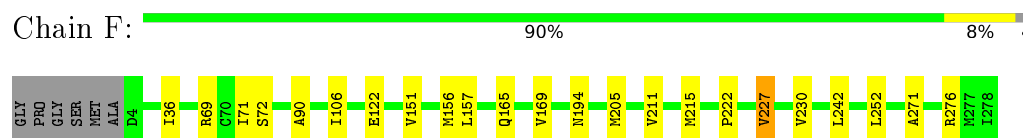
Chain D: 



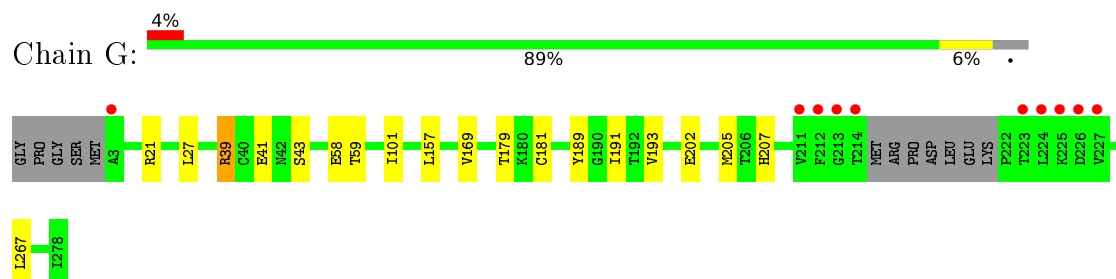
- Molecule 1: Putative short-chain dehydrogenase/reductase



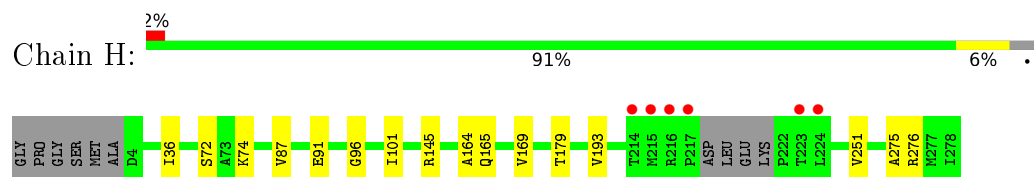
- Molecule 1: Putative short-chain dehydrogenase/reductase



- Molecule 1: Putative short-chain dehydrogenase/reductase



- Molecule 1: Putative short-chain dehydrogenase/reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.36 Å 84.97 Å 100.89 Å 81.77° 76.78° 74.23°	Depositor
Resolution (Å)	50.00 – 2.10 45.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.10) 92.2 (45.76-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.38 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.237 0.194 , 0.198	Depositor DCC
R_{free} test set	5997 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	11.6	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17342	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.40% 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: CA, NAD

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	0.67	0/1993	0.68	0/2715
1	B	0.67	0/2011	0.68	0/2739
1	C	0.66	0/1991	0.69	1/2712 (0.0%)
1	D	0.66	0/2022	0.68	1/2759 (0.0%)
1	E	0.68	0/1957	0.68	0/2665
1	F	0.67	0/2046	0.69	0/2787
1	G	0.71	0/1994	0.67	0/2714
1	H	0.67	0/2009	0.67	0/2738
All	All	0.67	0/16023	0.68	2/21829 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	76	ASP	CB-CG-OD1	5.67	123.40	118.30

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	1957	0	1935	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1972	0	1951	17	0
1	C	1955	0	1933	11	0
1	D	1987	0	1950	14	0
1	E	1922	0	1887	8	0
1	F	2011	0	1986	18	0
1	G	1955	0	1942	11	0
1	H	1969	0	1953	10	0
2	A	44	0	26	0	0
2	B	44	0	26	0	0
2	C	44	0	26	2	0
2	D	44	0	26	0	0
2	E	44	0	26	0	0
2	F	44	0	26	1	0
2	G	44	0	26	1	0
2	H	44	0	26	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	H	1	0	0	0	0
4	A	145	0	0	2	0
4	B	153	0	0	1	0
4	C	151	0	0	1	0
4	D	145	0	0	1	0
4	E	148	0	0	0	0
4	F	185	0	0	2	0
4	G	167	0	0	0	0
4	H	160	0	0	2	0
All	All	17342	0	15745	96	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 3.

All (96) 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:G:27:LEU:HD11	1:G:101:ILE:HD11	1.69	0.72
1:A:270:ASP:OD2	1:A:274[A]:THR:HG23	1.91	0.70
1:C:227:VAL:O	1:C:230:VAL:HG12	1.92	0.70
1:C:39:ARG:HG2	4:C:299:HOH:O	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ARG:HB3	4:D:1050:HOH:O	1.92	0.68
1:F:69:ARG:NH2	4:F:1124:HOH:O	2.27	0.68
1:D:216:ARG:N	1:D:217:PRO:HD3	2.09	0.67
1:F:227:VAL:O	1:F:230:VAL:HG12	1.98	0.64
1:A:159:HIS:HE1	1:A:274[A]:THR:HG22	1.65	0.61
1:C:27:LEU:HD11	1:C:101:ILE:HD11	1.82	0.61
1:E:25:VAL:O	1:E:29[A]:GLU:HG3	2.03	0.58
1:A:39:ARG:HE	1:A:41:GLU:HG3	1.68	0.58
1:E:243:LYS:HE2	1:E:244:PRO:HD2	1.86	0.57
1:B:71:ILE:CD1	1:B:90:ALA:HA	2.35	0.57
1:H:276:ARG:HD2	4:H:580:HOH:O	2.05	0.56
1:F:71:ILE:HD11	1:F:90:ALA:CB	2.36	0.56
1:E:87:VAL:O	1:E:91:GLU:HG3	2.06	0.55
1:F:276:ARG:HD2	4:F:813:HOH:O	2.05	0.55
1:G:205:MET:CE	2:G:279:NAD:H2D	2.37	0.55
1:H:96:GLY:HA3	1:H:145:ARG:CZ	2.36	0.55
1:B:106:ILE:CD1	1:B:122:GLU:HG3	2.39	0.53
1:F:151:VAL:HA	1:F:194:ASN:O	2.09	0.52
1:D:216:ARG:H	1:D:217:PRO:HD3	1.72	0.52
1:B:202:GLU:HG3	1:B:207:HIS:CE1	2.46	0.51
1:B:69:ARG:NH2	4:B:314:HOH:O	2.44	0.50
1:B:157:LEU:HB3	1:B:169:VAL:HG22	1.94	0.50
1:F:106:ILE:CD1	1:F:122:GLU:HG3	2.42	0.50
1:A:242:LEU:HD21	1:A:271:ALA:HB2	1.93	0.50
1:A:159:HIS:CE1	1:A:274[A]:THR:HG22	2.47	0.50
1:B:5:PHE:HD2	1:B:30:ALA:HB1	1.77	0.49
1:D:87:VAL:O	1:D:91:GLU:HG2	2.12	0.49
1:G:39:ARG:HD3	1:G:41:GLU:HG3	1.94	0.49
1:D:218:ASP:O	1:D:219:LEU:HB2	2.11	0.49
1:B:61:ALA:O	1:B:65:LYS:HG2	2.13	0.48
1:F:215:MET:HB2	1:F:227:VAL:HG22	1.93	0.48
1:F:227:VAL:O	1:F:230:VAL:CG1	2.61	0.48
1:B:102:THR:OG1	1:B:152:THR:HA	2.13	0.48
1:B:27:LEU:HD11	1:B:101[A]:ILE:HD11	1.95	0.48
1:B:116[A]:GLU:HG2	1:B:119:GLN:HB2	1.95	0.48
1:E:200:ASN:OD1	1:E:234:LEU:HD12	2.13	0.47
1:G:181:CYS:SG	1:H:169:VAL:HB	2.54	0.47
1:A:44:ASP:HB2	4:A:415:HOH:O	2.14	0.47
1:F:242:LEU:HD21	1:F:271:ALA:HB2	1.96	0.47
1:C:157:LEU:HB3	1:C:169:VAL:HG22	1.94	0.47
1:C:169:VAL:HB	1:D:181:CYS:SG	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:MET:CE	2:F:279:NAD:H2D	2.45	0.47
1:F:71:ILE:HD13	1:F:90:ALA:HA	1.95	0.47
1:A:39:ARG:NH2	4:A:583:HOH:O	2.46	0.47
1:F:157:LEU:HB3	1:F:169:VAL:HG22	1.96	0.47
1:F:71:ILE:HD11	1:F:90:ALA:HB2	1.97	0.47
1:B:106:ILE:HD11	1:B:122:GLU:HG3	1.97	0.47
1:F:71:ILE:CD1	1:F:90:ALA:HA	2.44	0.47
1:B:151:VAL:HA	1:B:194:ASN:O	2.14	0.46
1:B:71:ILE:HD13	1:B:90:ALA:HA	1.97	0.46
1:D:236:LEU:HB3	1:D:272:GLY:HA3	1.96	0.46
1:D:157:LEU:HB3	1:D:169:VAL:HG22	1.97	0.46
1:H:74:LYS:HE2	4:H:555:HOH:O	2.15	0.46
1:B:179:THR:HG23	1:B:193:VAL:HG12	1.96	0.46
1:E:36:ILE:O	1:E:72:SER:HA	2.15	0.46
1:E:264:GLY:HA3	1:H:275:ALA:HB2	1.97	0.46
1:G:21:ARG:HG3	1:G:59:THR:HG23	1.97	0.46
1:G:189:TYR:HB2	1:G:191:ILE:HD12	1.98	0.45
1:D:179:THR:HG23	1:D:193:VAL:HG12	1.99	0.45
1:G:179:THR:HG23	1:G:193:VAL:HG12	1.98	0.45
1:A:71:ILE:HD11	1:A:90:ALA:HB2	1.99	0.45
1:C:181:CYS:SG	1:D:169:VAL:HB	2.57	0.44
1:A:111:LEU:HG	1:A:164:ALA:HB2	1.98	0.44
1:B:5:PHE:HD2	1:B:30:ALA:CB	2.31	0.44
1:H:87:VAL:O	1:H:91:GLU:HG2	2.17	0.44
1:C:36:ILE:O	1:C:72:SER:HA	2.18	0.43
1:G:157:LEU:HB3	1:G:169:VAL:HG22	2.00	0.43
1:C:189:TYR:HB2	1:C:191:ILE:HD12	1.99	0.43
1:E:34:ILE:CG2	1:E:36:ILE:HG23	2.48	0.43
1:G:27:LEU:HD11	1:G:101:ILE:CD1	2.43	0.43
1:H:179:THR:HG23	1:H:193:VAL:HG12	2.00	0.43
1:H:36:ILE:O	1:H:72:SER:HA	2.19	0.42
1:B:36:ILE:O	1:B:72:SER:HA	2.19	0.42
1:B:242:LEU:HD21	1:B:271:ALA:HB2	2.02	0.42
1:C:179:THR:HG23	1:C:193:VAL:HG12	2.00	0.42
1:A:159:HIS:HE1	1:A:274[A]:THR:CG2	2.31	0.42
1:F:106:ILE:HD11	1:F:122:GLU:HG3	2.01	0.42
1:F:36:ILE:O	1:F:72:SER:HA	2.19	0.42
1:C:199:GLY:O	2:C:279:NAD:H4N	2.20	0.41
1:E:242:LEU:HD21	1:E:271:ALA:HB2	2.02	0.41
1:G:202:GLU:HG3	1:G:207:HIS:NE2	2.35	0.41
1:D:228:GLU:HG2	1:D:240:PRO:HG3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:MET:CE	2:C:279:NAD:H2D	2.50	0.41
1:F:165[A]:GLN:HB3	1:F:169:VAL:HG23	2.01	0.41
1:A:38:ASP:O	1:A:74:LYS:HA	2.21	0.41
1:G:21:ARG:NH2	1:G:58:GLU:OE2	2.45	0.41
1:D:219:LEU:HD21	1:D:226:ASP:HB3	2.04	0.40
1:F:211:VAL:O	1:F:215:MET:HG3	2.21	0.40
1:H:101[A]:ILE:HD13	1:H:251:VAL:HG11	2.02	0.40
1:D:13:THR:O	1:D:103:ASN:HB3	2.21	0.40
1:H:164:ALA:O	1:H:165:GLN:HG2	2.22	0.40
1:D:27:LEU:HD11	1:D:101:ILE:HD11	2.02	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	267/281 (95%)	256 (96%)	11 (4%)	0	100	100
1	B	269/281 (96%)	263 (98%)	6 (2%)	0	100	100
1	C	267/281 (95%)	258 (97%)	8 (3%)	1 (0%)	39	37
1	D	274/281 (98%)	261 (95%)	9 (3%)	4 (2%)	13	7
1	E	264/281 (94%)	255 (97%)	9 (3%)	0	100	100
1	F	274/281 (98%)	267 (97%)	7 (3%)	0	100	100
1	G	268/281 (95%)	261 (97%)	7 (3%)	0	100	100
1	H	270/281 (96%)	259 (96%)	11 (4%)	0	100	100
All	All	2153/2248 (96%)	2080 (97%)	68 (3%)	5 (0%)	52	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	PRO
1	D	219	LEU
1	D	215	MET
1	D	218	ASP
1	D	216	ARG

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	202/216 (94%)	200 (99%)	2 (1%)	82	87
1	B	204/216 (94%)	203 (100%)	1 (0%)	92	95
1	C	203/216 (94%)	199 (98%)	4 (2%)	63	68
1	D	204/216 (94%)	202 (99%)	2 (1%)	82	87
1	E	195/216 (90%)	194 (100%)	1 (0%)	92	95
1	F	209/216 (97%)	205 (98%)	4 (2%)	65	70
1	G	202/216 (94%)	199 (98%)	3 (2%)	72	78
1	H	203/216 (94%)	203 (100%)	0	100	100
All	All	1622/1728 (94%)	1605 (99%)	17 (1%)	80	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	214	THR
1	B	224	LEU
1	C	4	ASP
1	C	39	ARG
1	C	44	ASP
1	C	224	LEU
1	D	229	SER
1	D	252	LEU
1	E	267	LEU
1	F	156	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	222	PRO
1	F	227	VAL
1	F	252	LEU
1	G	39	ARG
1	G	43	SER
1	G	267	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	146	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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	279	-	42,48,48	0.72	0	46,73,73	1.79	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	B	279	-	42,48,48	0.73	0	46,73,73	1.60	3 (6%)
2	NAD	C	279	-	42,48,48	0.74	0	46,73,73	2.12	4 (8%)
2	NAD	D	279	-	42,48,48	0.74	0	46,73,73	2.05	4 (8%)
2	NAD	E	279	-	42,48,48	0.76	0	46,73,73	1.68	5 (10%)
2	NAD	F	279	-	42,48,48	0.71	0	46,73,73	1.88	6 (13%)
2	NAD	G	279	-	42,48,48	0.68	0	46,73,73	1.77	3 (6%)
2	NAD	H	279	-	42,48,48	0.79	2 (4%)	46,73,73	2.31	5 (10%)

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	279	-	-	0/22/62/62	0/5/5/5
2	NAD	B	279	-	-	0/22/62/62	0/5/5/5
2	NAD	C	279	-	-	0/22/62/62	0/5/5/5
2	NAD	D	279	-	-	0/22/62/62	0/5/5/5
2	NAD	E	279	-	-	0/22/62/62	0/5/5/5
2	NAD	F	279	-	-	0/22/62/62	0/5/5/5
2	NAD	G	279	-	-	0/22/62/62	0/5/5/5
2	NAD	H	279	-	-	0/22/62/62	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	279	NAD	C4A-N3A	2.09	1.38	1.35
2	H	279	NAD	O4D-C1D	2.33	1.44	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	279	NAD	N3A-C2A-N1A	-13.40	118.34	128.87
2	C	279	NAD	N3A-C2A-N1A	-11.73	119.65	128.87
2	D	279	NAD	N3A-C2A-N1A	-11.55	119.80	128.87
2	G	279	NAD	N3A-C2A-N1A	-10.04	120.99	128.87
2	F	279	NAD	N3A-C2A-N1A	-9.63	121.31	128.87
2	A	279	NAD	N3A-C2A-N1A	-9.17	121.67	128.87
2	E	279	NAD	N3A-C2A-N1A	-9.08	121.74	128.87
2	B	279	NAD	N3A-C2A-N1A	-8.05	122.55	128.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	279	NAD	C1B-N9A-C4A	-4.96	121.27	126.81
2	F	279	NAD	C1B-N9A-C4A	-4.80	121.45	126.81
2	H	279	NAD	C1B-N9A-C4A	-3.65	122.73	126.81
2	B	279	NAD	C1B-N9A-C4A	-3.26	123.17	126.81
2	D	279	NAD	C1B-N9A-C4A	-3.02	123.43	126.81
2	A	279	NAD	C1B-N9A-C4A	-3.01	123.44	126.81
2	E	279	NAD	C1B-N9A-C4A	-2.60	123.91	126.81
2	B	279	NAD	C4B-O4B-C1B	-2.52	106.97	109.64
2	F	279	NAD	O7N-C7N-N7N	-2.45	119.09	122.58
2	E	279	NAD	C3N-C7N-N7N	2.01	120.10	117.82
2	A	279	NAD	C2A-N1A-C6A	2.03	122.39	118.77
2	H	279	NAD	C2A-N1A-C6A	2.05	122.43	118.77
2	G	279	NAD	O2N-PN-O3	2.08	114.19	105.27
2	F	279	NAD	C3N-C7N-N7N	2.16	120.27	117.82
2	C	279	NAD	C2A-N1A-C6A	2.17	122.64	118.77
2	A	279	NAD	O4B-C1B-N9A	2.19	112.24	108.11
2	E	279	NAD	O2N-PN-O3	2.19	114.67	105.27
2	H	279	NAD	C3N-C7N-N7N	2.21	120.32	117.82
2	F	279	NAD	O4D-C1D-N1N	2.22	110.51	108.10
2	F	279	NAD	O2N-PN-O3	2.29	115.07	105.27
2	E	279	NAD	O4D-C1D-N1N	2.38	110.67	108.10
2	A	279	NAD	C3N-C7N-N7N	2.48	120.62	117.82
2	D	279	NAD	O2N-PN-O3	2.53	116.11	105.27
2	G	279	NAD	C3N-C7N-N7N	2.58	120.74	117.82
2	C	279	NAD	C3N-C7N-N7N	2.58	120.74	117.82
2	D	279	NAD	O4D-C1D-N1N	2.63	110.94	108.10
2	H	279	NAD	O4D-C1D-N1N	2.87	111.20	108.10
2	A	279	NAD	O4D-C1D-N1N	2.95	111.29	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	279	NAD	2	0
2	F	279	NAD	1	0
2	G	279	NAD	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	269/281 (95%)	-0.01	8 (2%)	54	62	4, 11, 29, 43	0
1	B	270/281 (96%)	-0.09	7 (2%)	59	66	3, 9, 28, 42	0
1	C	269/281 (95%)	-0.08	6 (2%)	65	71	3, 9, 29, 44	0
1	D	275/281 (97%)	-0.02	11 (4%)	42	51	4, 10, 36, 52	0
1	E	266/281 (94%)	-0.08	6 (2%)	64	70	3, 10, 29, 46	0
1	F	275/281 (97%)	-0.14	0	100	100	3, 9, 27, 35	0
1	G	269/281 (95%)	-0.12	10 (3%)	45	54	3, 9, 27, 41	0
1	H	271/281 (96%)	-0.03	6 (2%)	65	71	4, 10, 30, 45	0
All	All	2164/2248 (96%)	-0.07	54 (2%)	61	67	3, 10, 30, 52	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	214	THR	4.1
1	B	224	LEU	4.1
1	D	215	MET	3.9
1	D	218	ASP	3.9
1	D	213	GLY	3.7
1	C	221	LYS	3.3
1	D	217	PRO	3.3
1	G	213	GLY	3.2
1	B	223	THR	3.1
1	C	212	PHE	3.0
1	A	213	GLY	2.9
1	D	223	THR	2.9
1	E	214	THR	2.9
1	D	219	LEU	2.9
1	C	3	ALA	2.8
1	G	225	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	3	ALA	2.8
1	A	3	ALA	2.7
1	B	214	THR	2.7
1	B	211	VAL	2.7
1	E	69	ARG	2.7
1	H	224	LEU	2.7
1	H	215	MET	2.6
1	H	223	THR	2.6
1	C	222	PRO	2.5
1	E	3	ALA	2.5
1	A	210	PHE	2.5
1	G	224	LEU	2.5
1	H	214	THR	2.4
1	D	224	LEU	2.4
1	G	212	PHE	2.4
1	G	214	THR	2.4
1	D	220	GLU	2.4
1	A	224	LEU	2.3
1	B	213	GLY	2.3
1	A	223	THR	2.3
1	A	222	PRO	2.2
1	B	238	TYR	2.2
1	H	217	PRO	2.2
1	E	226	ASP	2.2
1	D	221	LYS	2.2
1	C	211	VAL	2.2
1	H	216	ARG	2.2
1	A	232	ALA	2.2
1	G	223	THR	2.2
1	A	231	PHE	2.1
1	G	226	ASP	2.1
1	G	211	VAL	2.1
1	G	227	VAL	2.1
1	C	229	SER	2.1
1	B	226	ASP	2.1
1	D	212	PHE	2.0
1	E	96	GLY	2.0
1	E	213	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	E	279	44/44	0.97	0.09	-0.61	6,9,11,11	0
2	NAD	F	279	44/44	0.97	0.09	-0.71	3,7,10,10	0
2	NAD	A	279	44/44	0.97	0.09	-0.74	6,10,13,14	0
2	NAD	G	279	44/44	0.97	0.09	-0.75	3,6,9,10	0
2	NAD	B	279	44/44	0.97	0.08	-0.87	4,7,9,10	0
2	NAD	D	279	44/44	0.97	0.09	-1.17	3,6,8,11	0
2	NAD	H	279	44/44	0.97	0.08	-1.25	3,7,9,11	0
2	NAD	C	279	44/44	0.97	0.09	-1.68	3,7,10,11	0
3	CA	F	280	1/1	0.95	0.06	-1.79	25,25,25,25	0
3	CA	F	281	1/1	0.99	0.07	-2.01	25,25,25,25	0
3	CA	A	280	1/1	0.99	0.07	-2.35	22,22,22,22	0
3	CA	D	280	1/1	0.95	0.06	-3.02	36,36,36,36	0
3	CA	B	280	1/1	0.98	0.05	-3.89	25,25,25,25	0
3	CA	B	281	1/1	0.96	0.07	-	30,30,30,30	0
3	CA	E	280	1/1	0.96	0.09	-	29,29,29,29	0
3	CA	H	280	1/1	0.97	0.04	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.