



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:59 PM GMT

PDB ID : 1ZBQ
Title : Crystal Structure Of Human 17-Beta-Hydroxysteroid Dehydrogenase Type 4
In Complex With NAD
Authors : Lukacik, P.; Shafqat, N.; Kavanagh, K.; Bray, J.; Von Delft, F.; Edwards,
A.; Arrowsmith, C.; Sundstrom, M.; Oppermann, U.; Structural Genomics
Consortium (SGC)
Deposited on : 2005-04-08
Resolution : 2.19 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
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)	:	trunk26865

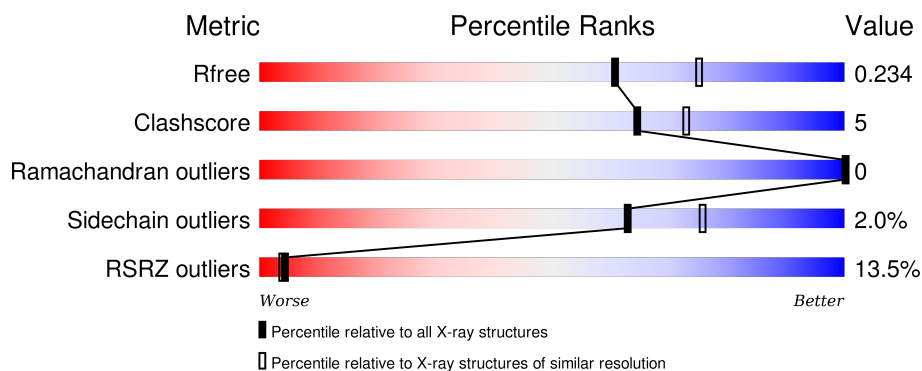
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>11%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	B	327	<div> <div>12%</div> <div>86%</div> <div>7%</div> <div>8%</div> </div>
1	C	327	<div> <div>12%</div> <div>80%</div> <div>11%</div> <div>8%</div> </div>
1	D	327	<div> <div>10%</div> <div>81%</div> <div>11%</div> <div>8%</div> </div>
1	E	327	<div> <div>17%</div> <div>84%</div> <div>9%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	327	<div><div></div><div>13%</div><div>84%</div><div>8%</div><div>8%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14189 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 17-beta-hydroxysteroid dehydrogenase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	2	0
			2267	1430	409	419	9			
1	B	302	Total	C	N	O	S	0	1	0
			2264	1427	410	418	9			
1	C	302	Total	C	N	O	S	0	1	0
			2268	1428	409	422	9			
1	D	302	Total	C	N	O	S	0	3	0
			2289	1442	419	419	9			
1	E	302	Total	C	N	O	S	0	1	0
			2235	1403	408	415	9			
1	F	302	Total	C	N	O	S	0	2	0
			2259	1418	407	425	9			

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	GLY	-	CLONING ARTIFACT	UNP P51659
A	-19	SER	-	CLONING ARTIFACT	UNP P51659
A	-18	SER	-	CLONING ARTIFACT	UNP P51659
A	-17	HIS	-	EXPRESSION TAG	UNP P51659
A	-16	HIS	-	EXPRESSION TAG	UNP P51659
A	-15	HIS	-	EXPRESSION TAG	UNP P51659
A	-14	HIS	-	EXPRESSION TAG	UNP P51659
A	-13	HIS	-	EXPRESSION TAG	UNP P51659
A	-12	HIS	-	EXPRESSION TAG	UNP P51659
A	-11	SER	-	CLONING ARTIFACT	UNP P51659
A	-10	SER	-	CLONING ARTIFACT	UNP P51659
A	-9	GLY	-	CLONING ARTIFACT	UNP P51659
A	-8	ARG	-	CLONING ARTIFACT	UNP P51659
A	-7	GLU	-	CLONING ARTIFACT	UNP P51659
A	-6	ASN	-	CLONING ARTIFACT	UNP P51659
A	-5	LEU	-	CLONING ARTIFACT	UNP P51659
A	-4	TYR	-	CLONING ARTIFACT	UNP P51659

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	CLONING ARTIFACT	UNP P51659
A	-2	GLN	-	CLONING ARTIFACT	UNP P51659
A	-1	GLY	-	CLONING ARTIFACT	UNP P51659
A	0	HIS	-	CLONING ARTIFACT	UNP P51659
A	305	GLY	-	CLONING ARTIFACT	UNP P51659
A	306	SER	-	CLONING ARTIFACT	UNP P51659
B	-20	GLY	-	CLONING ARTIFACT	UNP P51659
B	-19	SER	-	CLONING ARTIFACT	UNP P51659
B	-18	SER	-	CLONING ARTIFACT	UNP P51659
B	-17	HIS	-	EXPRESSION TAG	UNP P51659
B	-16	HIS	-	EXPRESSION TAG	UNP P51659
B	-15	HIS	-	EXPRESSION TAG	UNP P51659
B	-14	HIS	-	EXPRESSION TAG	UNP P51659
B	-13	HIS	-	EXPRESSION TAG	UNP P51659
B	-12	HIS	-	EXPRESSION TAG	UNP P51659
B	-11	SER	-	CLONING ARTIFACT	UNP P51659
B	-10	SER	-	CLONING ARTIFACT	UNP P51659
B	-9	GLY	-	CLONING ARTIFACT	UNP P51659
B	-8	ARG	-	CLONING ARTIFACT	UNP P51659
B	-7	GLU	-	CLONING ARTIFACT	UNP P51659
B	-6	ASN	-	CLONING ARTIFACT	UNP P51659
B	-5	LEU	-	CLONING ARTIFACT	UNP P51659
B	-4	TYR	-	CLONING ARTIFACT	UNP P51659
B	-3	PHE	-	CLONING ARTIFACT	UNP P51659
B	-2	GLN	-	CLONING ARTIFACT	UNP P51659
B	-1	GLY	-	CLONING ARTIFACT	UNP P51659
B	0	HIS	-	CLONING ARTIFACT	UNP P51659
B	305	GLY	-	CLONING ARTIFACT	UNP P51659
B	306	SER	-	CLONING ARTIFACT	UNP P51659
C	-20	GLY	-	CLONING ARTIFACT	UNP P51659
C	-19	SER	-	CLONING ARTIFACT	UNP P51659
C	-18	SER	-	CLONING ARTIFACT	UNP P51659
C	-17	HIS	-	EXPRESSION TAG	UNP P51659
C	-16	HIS	-	EXPRESSION TAG	UNP P51659
C	-15	HIS	-	EXPRESSION TAG	UNP P51659
C	-14	HIS	-	EXPRESSION TAG	UNP P51659
C	-13	HIS	-	EXPRESSION TAG	UNP P51659
C	-12	HIS	-	EXPRESSION TAG	UNP P51659
C	-11	SER	-	CLONING ARTIFACT	UNP P51659
C	-10	SER	-	CLONING ARTIFACT	UNP P51659
C	-9	GLY	-	CLONING ARTIFACT	UNP P51659
C	-8	ARG	-	CLONING ARTIFACT	UNP P51659

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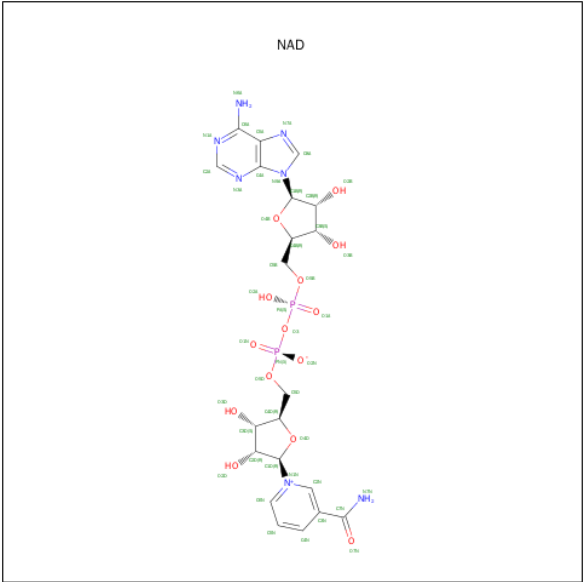
Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLU	-	CLONING ARTIFACT	UNP P51659
C	-6	ASN	-	CLONING ARTIFACT	UNP P51659
C	-5	LEU	-	CLONING ARTIFACT	UNP P51659
C	-4	TYR	-	CLONING ARTIFACT	UNP P51659
C	-3	PHE	-	CLONING ARTIFACT	UNP P51659
C	-2	GLN	-	CLONING ARTIFACT	UNP P51659
C	-1	GLY	-	CLONING ARTIFACT	UNP P51659
C	0	HIS	-	CLONING ARTIFACT	UNP P51659
C	305	GLY	-	CLONING ARTIFACT	UNP P51659
C	306	SER	-	CLONING ARTIFACT	UNP P51659
D	-20	GLY	-	CLONING ARTIFACT	UNP P51659
D	-19	SER	-	CLONING ARTIFACT	UNP P51659
D	-18	SER	-	CLONING ARTIFACT	UNP P51659
D	-17	HIS	-	EXPRESSION TAG	UNP P51659
D	-16	HIS	-	EXPRESSION TAG	UNP P51659
D	-15	HIS	-	EXPRESSION TAG	UNP P51659
D	-14	HIS	-	EXPRESSION TAG	UNP P51659
D	-13	HIS	-	EXPRESSION TAG	UNP P51659
D	-12	HIS	-	EXPRESSION TAG	UNP P51659
D	-11	SER	-	CLONING ARTIFACT	UNP P51659
D	-10	SER	-	CLONING ARTIFACT	UNP P51659
D	-9	GLY	-	CLONING ARTIFACT	UNP P51659
D	-8	ARG	-	CLONING ARTIFACT	UNP P51659
D	-7	GLU	-	CLONING ARTIFACT	UNP P51659
D	-6	ASN	-	CLONING ARTIFACT	UNP P51659
D	-5	LEU	-	CLONING ARTIFACT	UNP P51659
D	-4	TYR	-	CLONING ARTIFACT	UNP P51659
D	-3	PHE	-	CLONING ARTIFACT	UNP P51659
D	-2	GLN	-	CLONING ARTIFACT	UNP P51659
D	-1	GLY	-	CLONING ARTIFACT	UNP P51659
D	0	HIS	-	CLONING ARTIFACT	UNP P51659
D	305	GLY	-	CLONING ARTIFACT	UNP P51659
D	306	SER	-	CLONING ARTIFACT	UNP P51659
E	-20	GLY	-	CLONING ARTIFACT	UNP P51659
E	-19	SER	-	CLONING ARTIFACT	UNP P51659
E	-18	SER	-	CLONING ARTIFACT	UNP P51659
E	-17	HIS	-	EXPRESSION TAG	UNP P51659
E	-16	HIS	-	EXPRESSION TAG	UNP P51659
E	-15	HIS	-	EXPRESSION TAG	UNP P51659
E	-14	HIS	-	EXPRESSION TAG	UNP P51659
E	-13	HIS	-	EXPRESSION TAG	UNP P51659
E	-12	HIS	-	EXPRESSION TAG	UNP P51659

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-11	SER	-	CLONING ARTIFACT	UNP P51659
E	-10	SER	-	CLONING ARTIFACT	UNP P51659
E	-9	GLY	-	CLONING ARTIFACT	UNP P51659
E	-8	ARG	-	CLONING ARTIFACT	UNP P51659
E	-7	GLU	-	CLONING ARTIFACT	UNP P51659
E	-6	ASN	-	CLONING ARTIFACT	UNP P51659
E	-5	LEU	-	CLONING ARTIFACT	UNP P51659
E	-4	TYR	-	CLONING ARTIFACT	UNP P51659
E	-3	PHE	-	CLONING ARTIFACT	UNP P51659
E	-2	GLN	-	CLONING ARTIFACT	UNP P51659
E	-1	GLY	-	CLONING ARTIFACT	UNP P51659
E	0	HIS	-	CLONING ARTIFACT	UNP P51659
E	305	GLY	-	CLONING ARTIFACT	UNP P51659
E	306	SER	-	CLONING ARTIFACT	UNP P51659
F	-20	GLY	-	CLONING ARTIFACT	UNP P51659
F	-19	SER	-	CLONING ARTIFACT	UNP P51659
F	-18	SER	-	CLONING ARTIFACT	UNP P51659
F	-17	HIS	-	EXPRESSION TAG	UNP P51659
F	-16	HIS	-	EXPRESSION TAG	UNP P51659
F	-15	HIS	-	EXPRESSION TAG	UNP P51659
F	-14	HIS	-	EXPRESSION TAG	UNP P51659
F	-13	HIS	-	EXPRESSION TAG	UNP P51659
F	-12	HIS	-	EXPRESSION TAG	UNP P51659
F	-11	SER	-	CLONING ARTIFACT	UNP P51659
F	-10	SER	-	CLONING ARTIFACT	UNP P51659
F	-9	GLY	-	CLONING ARTIFACT	UNP P51659
F	-8	ARG	-	CLONING ARTIFACT	UNP P51659
F	-7	GLU	-	CLONING ARTIFACT	UNP P51659
F	-6	ASN	-	CLONING ARTIFACT	UNP P51659
F	-5	LEU	-	CLONING ARTIFACT	UNP P51659
F	-4	TYR	-	CLONING ARTIFACT	UNP P51659
F	-3	PHE	-	CLONING ARTIFACT	UNP P51659
F	-2	GLN	-	CLONING ARTIFACT	UNP P51659
F	-1	GLY	-	CLONING ARTIFACT	UNP P51659
F	0	HIS	-	CLONING ARTIFACT	UNP P51659
F	305	GLY	-	CLONING ARTIFACT	UNP P51659
F	306	SER	-	CLONING ARTIFACT	UNP P51659

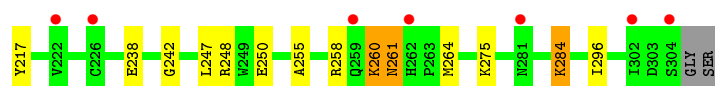
- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



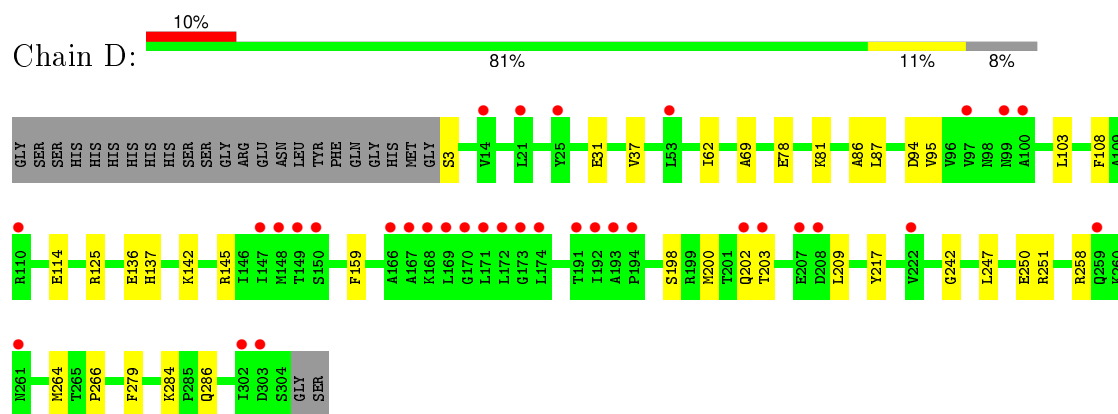
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is water.

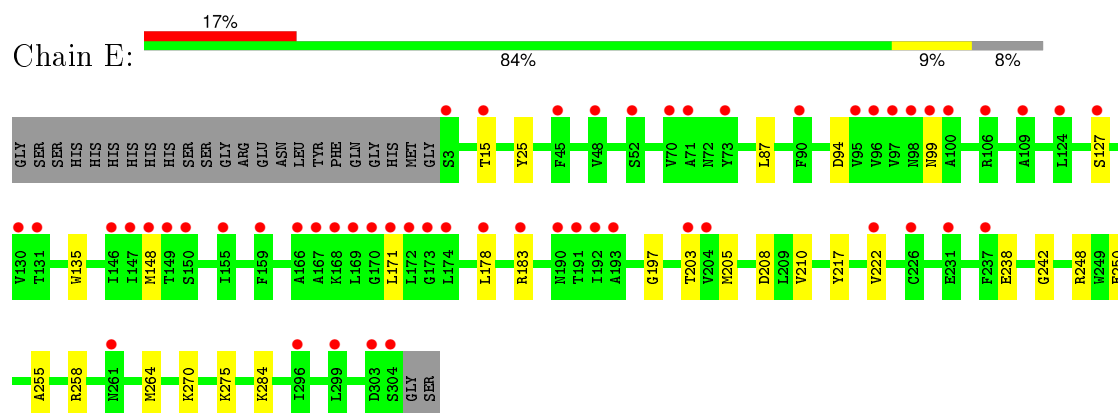
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	67	Total	O	0	0
			67	67		
3	C	66	Total	O	0	0
			66	66		
3	D	64	Total	O	0	0
			64	64		
3	E	42	Total	O	0	0
			42	42		
3	F	43	Total	O	0	0
			43	43		



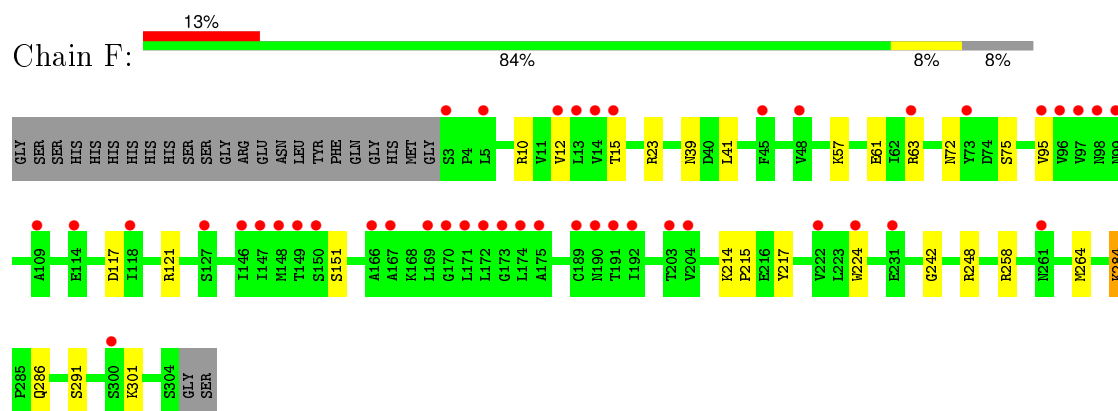
- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 4



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 4



- Molecule 1: 17-beta-hydroxysteroid dehydrogenase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.83Å 50.77Å 183.78Å 87.52° 87.07° 70.75°	Depositor
Resolution (Å)	50.57 – 2.19 32.68 – 2.19	Depositor EDS
% Data completeness (in resolution range)	76.2 (50.57-2.19) 75.8 (32.68-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.236 0.186 , 0.234	Depositor DCC
R_{free} test set	3383 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.2	EDS
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 67918 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14189	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.59	0/2310	0.65	0/3126
1	B	0.62	0/2307	0.67	0/3120
1	C	0.62	0/2311	0.67	1/3128 (0.0%)
1	D	0.58	1/2339 (0.0%)	0.67	1/3159 (0.0%)
1	E	0.53	0/2278	0.61	0/3089
1	F	0.61	2/2305 (0.1%)	0.65	2/3124 (0.1%)
All	All	0.59	3/13850 (0.0%)	0.65	4/18746 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	ARG	CZ-NH1	9.30	1.45	1.33
1	F	10	ARG	NE-CZ	5.88	1.40	1.33
1	D	250	GLU	CB-CG	-5.08	1.42	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	63	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	F	63	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	94	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	53	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	260	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2267	0	2227	31	0
1	B	2264	0	2226	24	0
1	C	2268	0	2229	38	0
1	D	2289	0	2282	27	0
1	E	2235	0	2158	32	0
1	F	2259	0	2184	22	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	1	0
2	F	44	0	26	0	0
3	A	61	0	0	1	0
3	B	67	0	0	2	0
3	C	66	0	0	0	0
3	D	64	0	0	2	0
3	E	42	0	0	0	0
3	F	43	0	0	2	0
All	All	14189	0	13462	139	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 5.

The worst 5 of 139 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:258:ARG:HB2	1:E:264:MET:HE2	1.46	0.94
1:E:264:MET:CE	1:F:242:GLY:HA2	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:MET:HE1	1:E:171:LEU:HD22	1.57	0.86
1:F:258:ARG:HB2	1:F:264:MET:HE2	1.58	0.85
1:E:264:MET:HE1	1:F:242:GLY:HA2	1.58	0.83

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	302/327 (92%)	295 (98%)	7 (2%)	0	100	100
1	B	301/327 (92%)	297 (99%)	4 (1%)	0	100	100
1	C	301/327 (92%)	296 (98%)	5 (2%)	0	100	100
1	D	303/327 (93%)	296 (98%)	7 (2%)	0	100	100
1	E	301/327 (92%)	294 (98%)	7 (2%)	0	100	100
1	F	302/327 (92%)	296 (98%)	6 (2%)	0	100	100
All	All	1810/1962 (92%)	1774 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	222/258 (86%)	216 (97%)	6 (3%)	52	64
1	B	222/258 (86%)	220 (99%)	2 (1%)	84	92
1	C	225/258 (87%)	220 (98%)	5 (2%)	60	72
1	D	229/258 (89%)	222 (97%)	7 (3%)	47	59
1	E	216/258 (84%)	212 (98%)	4 (2%)	65	77
1	F	221/258 (86%)	218 (99%)	3 (1%)	74	85
All	All	1335/1548 (86%)	1308 (98%)	27 (2%)	63	76

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	284	LYS
1	D	114	GLU
1	F	284	LYS
1	D	3	SER
1	A	203	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	141	GLN
1	C	195	ASN
1	E	137	HIS
1	C	137	HIS
1	D	137	HIS

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

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAD	A	1001	-	38,48,48	1.74	3 (7%)	47,73,73	2.20	6 (12%)
2	NAD	B	1002	-	38,48,48	1.59	3 (7%)	47,73,73	2.40	8 (17%)
2	NAD	C	1003	-	38,48,48	1.62	3 (7%)	47,73,73	2.31	7 (14%)
2	NAD	D	1004	-	38,48,48	1.67	4 (10%)	47,73,73	2.23	7 (14%)
2	NAD	E	1005	-	38,48,48	1.66	3 (7%)	47,73,73	2.39	7 (14%)
2	NAD	F	1006	-	38,48,48	1.68	3 (7%)	47,73,73	2.25	7 (14%)

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	1001	-	-	0/22/62/62	0/5/5/5
2	NAD	B	1002	-	-	0/22/62/62	0/5/5/5
2	NAD	C	1003	-	-	0/22/62/62	0/5/5/5
2	NAD	D	1004	-	-	0/22/62/62	0/5/5/5
2	NAD	E	1005	-	-	0/22/62/62	0/5/5/5
2	NAD	F	1006	-	-	0/22/62/62	0/5/5/5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	NAD	PA-O2A	-2.09	1.46	1.54
2	D	1004	NAD	PN-O2N	-2.03	1.46	1.54
2	E	1005	NAD	C2A-N1A	2.33	1.38	1.33
2	C	1003	NAD	C2A-N1A	2.37	1.38	1.33
2	D	1004	NAD	C2A-N1A	2.61	1.38	1.33

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1005	NAD	N3A-C2A-N1A	-13.90	118.25	128.89
2	B	1002	NAD	N3A-C2A-N1A	-13.65	118.44	128.89
2	C	1003	NAD	N3A-C2A-N1A	-12.84	119.06	128.89
2	F	1006	NAD	N3A-C2A-N1A	-12.84	119.06	128.89
2	A	1001	NAD	N3A-C2A-N1A	-11.96	119.74	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1005	NAD	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	302/327 (92%)	0.73	36 (11%) 6 6	33, 39, 47, 54	0
1	B	302/327 (92%)	0.76	38 (12%) 5 5	33, 39, 47, 54	0
1	C	302/327 (92%)	0.71	39 (12%) 5 4	32, 39, 46, 54	0
1	D	302/327 (92%)	0.71	34 (11%) 7 6	33, 39, 47, 54	1 (0%)
1	E	302/327 (92%)	0.95	54 (17%) 2 2	33, 39, 47, 54	0
1	F	302/327 (92%)	0.92	44 (14%) 3 3	33, 39, 47, 54	0
All	All	1812/1962 (92%)	0.80	245 (13%) 4 4	32, 39, 47, 54	1 (0%)

The worst 5 of 245 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	147	ILE	5.9
1	F	97	VAL	5.8
1	B	147	ILE	5.7
1	E	169	LEU	5.6
1	E	147	ILE	5.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	E	1005	44/44	0.95	0.11	-0.87	31,37,40,41	0
2	NAD	F	1006	44/44	0.95	0.11	-1.08	28,34,42,45	0
2	NAD	B	1002	44/44	0.96	0.10	-1.12	20,28,31,33	0
2	NAD	C	1003	44/44	0.97	0.08	-1.41	21,27,31,32	0
2	NAD	D	1004	44/44	0.96	0.09	-1.44	25,30,32,34	0
2	NAD	A	1001	44/44	0.96	0.09	-1.67	22,27,33,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.