



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:37 AM GMT

PDB ID : 2NAC
Title : HIGH RESOLUTION STRUCTURES OF HOLO AND APO FORMATE DE-HYDROGENASE
Authors : Lamzin, V.S.; Dauter, Z.; Popov, V.O.; Harutyunyan, E.H.; Wilson, K.S.
Deposited on : 1994-07-06
Resolution : 1.80 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 (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

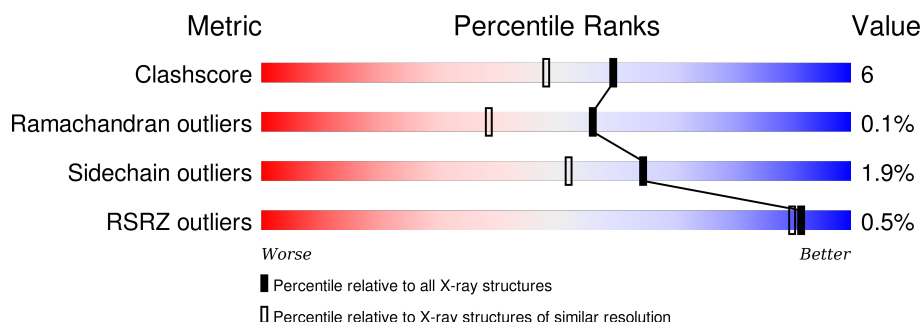
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	393	
1	B	393	

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	SO4	A	401	-	-	-	X
2	SO4	B	402	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6713 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 NAD-DEPENDENT FORMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	0	0
			2920	1850	512	544	14			
1	B	374	Total	C	N	O	S	0	0	0
			2920	1850	512	544	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

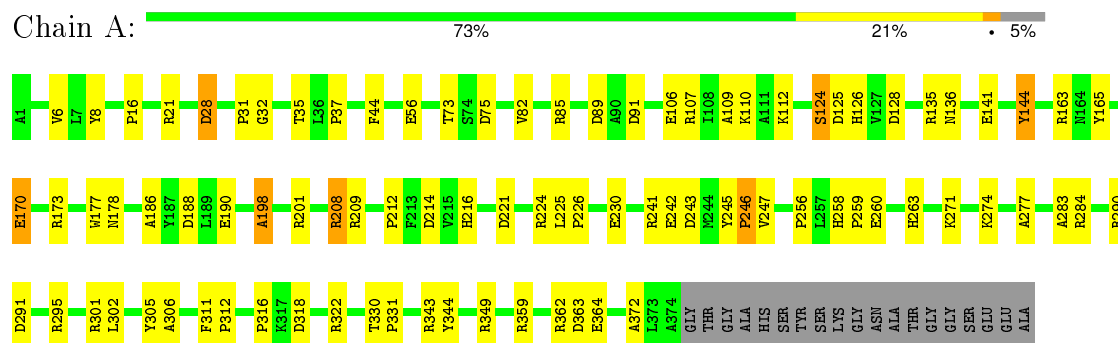
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	476	Total 476	O 476	0	0
3	B	387	Total 387	O 387	0	0

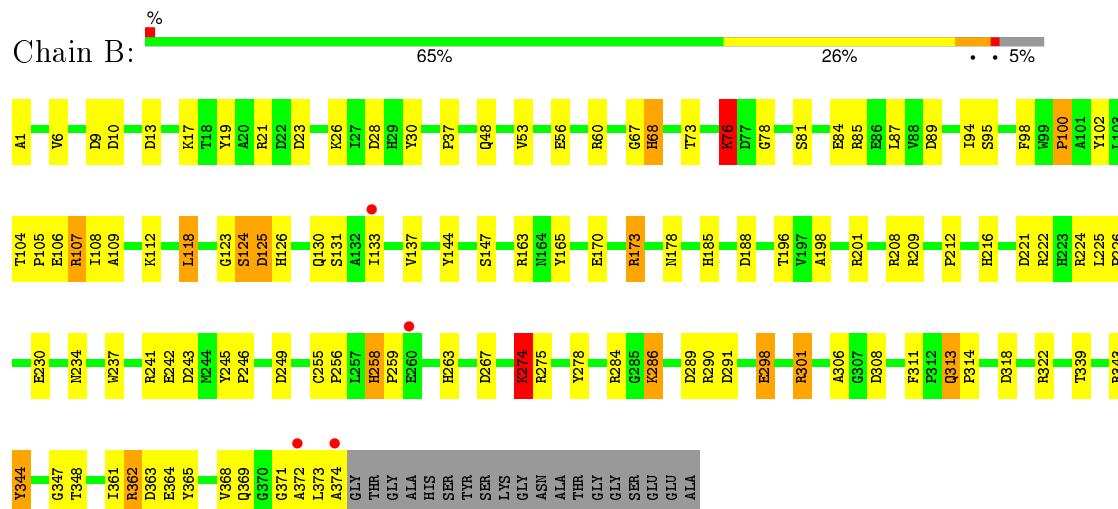
3 Residue-property plots

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: NAD-DEPENDENT FORMATE DEHYDROGENASE



• Molecule 1: NAD-DEPENDENT FORMATE DEHYDROGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	110.46 Å 54.47 Å 70.29 Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 9.98 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 97.2 (9.98-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.84 (at 1.80 Å)	Xtriage
Refinement program	ARP/WARP, PROLSQ	Depositor
R, R_{free}	0.146 , (Not available) 0.145 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 73563 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6713	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	1/2994 (0.0%)	2.02	89/4083 (2.2%)
1	B	1.03	1/2994 (0.0%)	2.16	111/4083 (2.7%)
All	All	1.04	2/5988 (0.0%)	2.09	200/8166 (2.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	GLU	CD-OE2	-5.22	1.20	1.25
1	B	9	ASP	CB-CG	5.09	1.62	1.51

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	222	ARG	CD-NE-CZ	20.26	151.96	123.60
1	B	21	ARG	NE-CZ-NH2	-19.59	110.51	120.30
1	B	173	ARG	NE-CZ-NH1	18.81	129.71	120.30
1	B	275	ARG	NE-CZ-NH2	-18.28	111.16	120.30
1	B	201	ARG	NE-CZ-NH2	-17.16	111.72	120.30
1	B	9	ASP	CB-CG-OD2	-17.15	102.86	118.30
1	A	201	ARG	NE-CZ-NH1	16.36	128.48	120.30
1	A	243	ASP	CB-CG-OD2	15.05	131.85	118.30
1	A	201	ARG	NE-CZ-NH2	-14.27	113.16	120.30
1	A	21	ARG	NE-CZ-NH2	-14.05	113.28	120.30
1	B	60	ARG	NE-CZ-NH2	14.04	127.32	120.30
1	A	362	ARG	NE-CZ-NH2	-13.67	113.46	120.30
1	B	343	ARG	NE-CZ-NH1	-12.17	114.22	120.30
1	A	274	LYS	CA-CB-CG	11.76	139.28	113.40
1	B	208	ARG	CD-NE-CZ	11.74	140.04	123.60
1	B	13	ASP	CB-CG-OD1	11.50	128.65	118.30
1	A	284	ARG	CD-NE-CZ	11.47	139.65	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	ARG	NE-CZ-NH1	11.27	125.94	120.30
1	B	107	ARG	NE-CZ-NH1	-11.13	114.73	120.30
1	A	208	ARG	NE-CZ-NH1	10.64	125.62	120.30
1	A	349	ARG	NE-CZ-NH1	-10.63	114.99	120.30
1	A	318	ASP	CB-CG-OD1	10.38	127.65	118.30
1	A	85	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	B	249	ASP	CB-CG-OD1	-10.37	108.97	118.30
1	B	222	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	107	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	B	13	ASP	CB-CG-OD2	-10.07	109.24	118.30
1	B	301	ARG	NE-CZ-NH2	-10.05	115.28	120.30
1	B	362	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	B	209	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	B	291	ASP	CB-CG-OD2	-9.95	109.35	118.30
1	B	363	ASP	CB-CG-OD1	9.82	127.14	118.30
1	B	201	ARG	NH1-CZ-NH2	9.52	129.87	119.40
1	A	56	GLU	OE1-CD-OE2	9.50	134.70	123.30
1	B	173	ARG	NH1-CZ-NH2	-9.47	108.98	119.40
1	B	28	ASP	CB-CA-C	-9.47	91.47	110.40
1	B	21	ARG	NH1-CZ-NH2	9.40	129.74	119.40
1	A	165	TYR	CB-CG-CD1	9.28	126.57	121.00
1	A	295	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	311	PHE	CB-CG-CD1	-9.08	114.44	120.80
1	B	301	ARG	CD-NE-CZ	8.79	135.90	123.60
1	A	214	ASP	CB-CG-OD1	8.74	126.17	118.30
1	A	284	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	B	173	ARG	CD-NE-CZ	8.71	135.79	123.60
1	A	322	ARG	NE-CZ-NH2	8.69	124.65	120.30
1	B	208	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	A	163	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	A	107	ARG	NH1-CZ-NH2	8.27	128.50	119.40
1	B	85	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	107	ARG	NE-CZ-NH1	-8.25	116.17	120.30
1	A	221	ASP	CB-CG-OD1	8.19	125.67	118.30
1	B	60	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	B	275	ARG	NH1-CZ-NH2	8.15	128.37	119.40
1	A	21	ARG	NH1-CZ-NH2	8.14	128.36	119.40
1	B	322	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	B	221	ASP	CB-CG-OD1	8.03	125.53	118.30
1	B	291	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	291	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	144	TYR	CB-CG-CD2	7.77	125.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	A	173	ARG	CD-NE-CZ	7.75	134.45	123.60
1	B	60	ARG	CD-NE-CZ	7.69	134.36	123.60
1	A	188	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	B	343	ARG	NH1-CZ-NH2	7.55	127.71	119.40
1	A	8	TYR	CB-CG-CD1	7.54	125.53	121.00
1	B	222	ARG	CG-CD-NE	7.49	127.53	111.80
1	A	173	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	91	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	A	85	ARG	NH1-CZ-NH2	7.46	127.61	119.40
1	A	359	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	B	84	GLU	CA-CB-CG	-7.39	97.15	113.40
1	A	89	ASP	CB-CG-OD1	-7.38	111.65	118.30
1	B	9	ASP	OD1-CG-OD2	7.33	137.24	123.30
1	B	100	PRO	O-C-N	7.32	134.41	122.70
1	A	221	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	364	GLU	OE1-CD-OE2	7.24	131.99	123.30
1	B	95	SER	N-CA-CB	7.22	121.33	110.50
1	B	10	ASP	CB-CG-OD1	7.21	124.78	118.30
1	B	242	GLU	OE1-CD-OE2	7.12	131.84	123.30
1	A	301	ARG	CD-NE-CZ	7.10	133.54	123.60
1	A	28	ASP	N-CA-CB	7.07	123.32	110.60
1	A	344	TYR	CB-CG-CD2	-6.99	116.81	121.00
1	B	290	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	75	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	124	SER	N-CA-CB	-6.88	100.18	110.50
1	B	301	ARG	NH1-CZ-NH2	6.88	126.97	119.40
1	A	290	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	B	289	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	28	ASP	CB-CA-C	-6.81	96.78	110.40
1	A	91	ASP	CB-CG-OD2	6.79	124.41	118.30
1	A	343	ARG	NE-CZ-NH1	-6.78	116.91	120.30
1	B	84	GLU	CG-CD-OE2	-6.71	104.89	118.30
1	B	198	ALA	N-CA-CB	6.64	119.40	110.10
1	B	318	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	224	ARG	CG-CD-NE	-6.43	98.29	111.80
1	A	260	GLU	OE1-CD-OE2	6.42	131.01	123.30
1	B	85	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	B	84	GLU	CG-CD-OE1	6.37	131.05	118.30
1	B	369	GLN	CA-CB-CG	-6.35	99.42	113.40
1	A	260	GLU	N-CA-CB	-6.33	99.20	110.60
1	A	209	ARG	NE-CZ-NH1	-6.31	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	344	TYR	CA-CB-CG	6.30	125.36	113.40
1	A	125	ASP	CB-CA-C	6.28	122.96	110.40
1	B	165	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	A	283	ALA	CB-CA-C	6.27	119.51	110.10
1	A	230	GLU	OE1-CD-OE2	-6.26	115.79	123.30
1	B	249	ASP	OD1-CG-OD2	6.24	135.16	123.30
1	B	188	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	A	28	ASP	CB-CG-OD2	-6.17	112.74	118.30
1	B	23	ASP	CB-CG-OD1	6.16	123.85	118.30
1	B	298	GLU	CA-CB-CG	6.15	126.93	113.40
1	B	56	GLU	OE1-CD-OE2	6.12	130.65	123.30
1	A	85	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	362	ARG	NH1-CZ-NH2	6.09	126.10	119.40
1	A	344	TYR	CB-CG-CD1	6.05	124.63	121.00
1	B	125	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	128	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	94	ILE	O-C-N	-5.98	113.13	122.70
1	B	208	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	372	ALA	O-C-N	5.91	132.15	122.70
1	A	291	ASP	CB-CG-OD1	5.88	123.59	118.30
1	B	298	GLU	OE1-CD-OE2	5.88	130.36	123.30
1	A	16	PRO	N-CA-CB	5.87	110.34	103.30
1	B	23	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	85	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	37	PRO	N-CA-CB	5.84	110.31	103.30
1	A	344	TYR	CA-CB-CG	5.79	124.41	113.40
1	A	243	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	B	313	GLN	N-CA-CB	-5.77	100.21	110.60
1	A	363	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	349	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	B	284	ARG	NH1-CZ-NH2	-5.71	113.12	119.40
1	A	170	GLU	CG-CD-OE1	-5.67	106.97	118.30
1	B	291	ASP	O-C-N	5.63	131.71	122.70
1	B	68	HIS	N-CA-CB	5.62	120.71	110.60
1	B	19	TYR	CB-CG-CD2	-5.61	117.63	121.00
1	B	165	TYR	CB-CG-CD1	5.56	124.34	121.00
1	A	198	ALA	N-CA-CB	5.56	117.88	110.10
1	B	365	TYR	CD1-CE1-CZ	5.55	124.80	119.80
1	B	107	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	B	123	GLY	O-C-N	5.55	131.57	122.70
1	B	125	ASP	CB-CG-OD1	-5.54	113.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	HIS	CB-CA-C	-5.50	99.40	110.40
1	A	82	VAL	CA-CB-CG1	5.49	119.14	110.90
1	A	302	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	78	GLY	CA-C-O	5.48	130.47	120.60
1	B	318	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	364	GLU	CG-CD-OE1	-5.44	107.42	118.30
1	A	35	THR	CA-CB-CG2	-5.42	104.82	112.40
1	B	278	TYR	CB-CG-CD2	5.41	124.24	121.00
1	B	267	ASP	CB-CG-OD1	5.39	123.16	118.30
1	B	30	TYR	CB-CG-CD1	5.38	124.23	121.00
1	A	241	ARG	CG-CD-NE	5.38	123.10	111.80
1	A	178	ASN	N-CA-CB	-5.38	100.92	110.60
1	A	32	GLY	CA-C-O	-5.37	110.93	120.60
1	A	186	ALA	N-CA-CB	5.37	117.62	110.10
1	B	308	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	177	TRP	CB-CA-C	5.36	121.13	110.40
1	A	318	ASP	OD1-CG-OD2	-5.36	113.11	123.30
1	B	76	LYS	CB-CG-CD	5.35	125.50	111.60
1	A	256	PRO	N-CA-CB	5.34	109.71	103.30
1	B	81	SER	N-CA-CB	-5.29	102.56	110.50
1	B	137	VAL	O-C-N	5.29	131.16	122.70
1	B	48	GLN	CG-CD-NE2	-5.29	104.02	116.70
1	A	277	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	246	PRO	N-CA-CB	5.26	109.62	103.30
1	B	196	THR	CA-CB-CG2	5.25	119.76	112.40
1	B	147	SER	O-C-N	5.25	131.09	122.70
1	B	339	THR	CA-CB-CG2	-5.24	105.06	112.40
1	A	242	GLU	CG-CD-OE2	-5.21	107.88	118.30
1	A	306	ALA	O-C-N	5.20	132.04	123.20
1	B	274	LYS	CB-CA-C	-5.19	100.02	110.40
1	B	89	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	295	ARG	NH1-CZ-NH2	5.18	125.10	119.40
1	B	278	TYR	CG-CD2-CE2	5.18	125.44	121.30
1	A	28	ASP	O-C-N	5.18	130.98	122.70
1	B	68	HIS	O-C-N	5.18	130.98	122.70
1	B	124	SER	O-C-N	-5.17	114.42	122.70
1	A	316	PRO	N-CA-CB	5.17	109.50	103.30
1	A	44	PHE	CB-CG-CD1	5.16	124.41	120.80
1	B	89	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	A	305	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	230	GLU	CG-CD-OE2	5.13	128.55	118.30
1	B	241	ARG	NE-CZ-NH2	-5.12	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	LYS	CA-CB-CG	-5.11	102.16	113.40
1	B	301	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	30	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	B	102	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	B	178	ASN	N-CA-CB	-5.09	101.43	110.60
1	B	374	ALA	N-CA-CB	-5.09	102.97	110.10
1	B	163	ARG	NH1-CZ-NH2	5.07	124.98	119.40
1	A	32	GLY	CA-C-N	5.07	126.34	116.20
1	A	31	PRO	N-CA-CB	5.05	109.36	103.30
1	A	190	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	B	372	ALA	CA-C-N	-5.05	106.09	117.20
1	B	28	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	53	VAL	CG1-CB-CG2	-5.04	102.84	110.90
1	B	241	ARG	CG-CD-NE	-5.03	101.23	111.80
1	B	306	ALA	N-CA-CB	5.02	117.13	110.10

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	2920	0	2876	20	0
1	B	2920	0	2876	46	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
3	A	476	0	0	8	4
3	B	387	0	0	19	4
All	All	6713	0	5752	66	7

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 6.

All (66) 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:A:135:ARG:NH1	3:A:632:HOH:O	2.04	0.91
1:B:124:SER:HB3	3:B:594:HOH:O	1.78	0.83
1:B:301:ARG:HB2	3:B:525:HOH:O	1.80	0.81
1:A:258:HIS:HB3	1:A:259:PRO:HD2	1.68	0.75
1:B:243:ASP:OD2	3:B:568:HOH:O	2.06	0.72
1:A:106:GLU:O	1:A:110:LYS:HG3	1.90	0.72
1:B:234:ASN:HB3	3:B:647:HOH:O	1.90	0.71
1:B:67:GLY:O	3:B:684:HOH:O	2.14	0.65
2:B:402:SO4:O3	3:B:451:HOH:O	2.11	0.65
1:A:225:LEU:HB3	1:A:226:PRO:HD2	1.79	0.64
1:B:368:VAL:HG22	1:B:373:LEU:HD23	1.78	0.64
1:B:258:HIS:HB3	1:B:259:PRO:CD	2.28	0.63
1:B:87:LEU:HD21	1:B:107:ARG:HB3	1.79	0.62
1:B:104:THR:O	1:B:108:ILE:HG13	2.01	0.61
1:A:170:GLU:HG3	3:B:750:HOH:O	2.00	0.59
1:B:124:SER:N	3:B:594:HOH:O	2.36	0.59
1:A:258:HIS:CB	1:A:259:PRO:HD2	2.31	0.57
1:B:313:GLN:HA	1:B:314:PRO:C	2.25	0.57
1:A:245:TYR:HB2	1:A:246:PRO:HD3	1.88	0.56
1:A:109:ALA:O	1:A:112:LYS:HE3	2.06	0.56
1:B:98:PHE:HE2	3:B:735:HOH:O	1.88	0.56
1:B:225:LEU:HB3	1:B:226:PRO:HD2	1.88	0.54
1:A:124:SER:HB2	3:A:565:HOH:O	2.08	0.53
1:B:104:THR:HB	1:B:105:PRO:HD2	1.91	0.51
1:A:212:PRO:HG3	1:B:212:PRO:HG3	1.92	0.51
1:B:124:SER:CB	3:B:594:HOH:O	2.49	0.51
3:A:537:HOH:O	1:B:216:HIS:HE1	1.94	0.51
1:A:208:ARG:NE	3:A:534:HOH:O	2.43	0.51
1:B:17:LYS:HE2	3:B:668:HOH:O	2.11	0.50
1:A:258:HIS:HB3	1:A:259:PRO:CD	2.40	0.50
1:B:126:HIS:H	1:B:126:HIS:CD2	2.29	0.49
1:B:255:CYS:HB2	1:B:256:PRO:HD2	1.95	0.49
1:A:126:HIS:CD2	1:A:126:HIS:H	2.31	0.49
1:A:271:LYS:NZ	3:A:557:HOH:O	2.16	0.48
1:A:216:HIS:HD2	3:A:601:HOH:O	1.96	0.48
1:B:298:GLU:HG3	3:B:780:HOH:O	2.13	0.48
1:B:124:SER:CA	3:B:594:HOH:O	2.61	0.47
1:B:170:GLU:CD	1:B:173:ARG:HH21	2.18	0.46
1:B:258:HIS:HB3	1:B:259:PRO:HD2	1.94	0.46
1:B:234:ASN:ND2	3:B:647:HOH:O	2.48	0.46
1:B:105:PRO:HB3	1:B:131:SER:OG	2.15	0.46
1:B:118:LEU:HD13	1:B:348:THR:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:831:HOH:O	1:B:173:ARG:HG3	2.16	0.45
1:B:274:LYS:HE2	3:B:579:HOH:O	2.16	0.45
1:A:311:PHE:HA	1:A:312:PRO:HA	1.79	0.44
1:B:1:ALA:O	1:B:68:HIS:HB3	2.18	0.44
1:B:17:LYS:H	1:B:17:LYS:HG2	1.47	0.44
1:B:361:ILE:O	1:B:362:ARG:C	2.55	0.44
1:B:133:ILE:O	1:B:371:GLY:HA2	2.18	0.43
1:B:245:TYR:HB2	1:B:246:PRO:HD3	2.00	0.43
1:A:216:HIS:HE1	3:B:502:HOH:O	2.02	0.43
1:B:224:ARG:HG2	1:B:237:TRP:CD2	2.53	0.43
1:B:6:VAL:HA	1:B:73:THR:O	2.19	0.43
1:B:106:GLU:O	1:B:109:ALA:HB3	2.18	0.43
1:B:112:LYS:HB2	3:B:703:HOH:O	2.19	0.43
1:B:76:LYS:HE2	1:B:100:PRO:O	2.19	0.42
1:A:6:VAL:HA	1:A:73:THR:O	2.19	0.42
1:B:216:HIS:HD2	3:B:569:HOH:O	2.01	0.42
1:B:185:HIS:HE1	3:B:450:HOH:O	2.03	0.42
1:B:26:LYS:HB3	1:B:26:LYS:HE2	1.93	0.41
1:B:6:VAL:HG11	1:B:76:LYS:HG3	2.02	0.41
1:A:247:VAL:HB	3:A:751:HOH:O	2.19	0.41
1:B:108:ILE:HD12	1:B:131:SER:HB2	2.03	0.41
1:B:130:GLN:O	1:B:133:ILE:HB	2.21	0.41
1:B:37:PRO:HB3	1:B:347:GLY:HA2	2.03	0.40
1:A:330:THR:HB	1:A:331:PRO:CD	2.52	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:528:HOH:O	3:A:563:HOH:O[2_657]	2.04	0.16
3:B:479:HOH:O	3:B:528:HOH:O[2_556]	2.05	0.15
3:A:524:HOH:O	3:A:528:HOH:O[2_647]	2.06	0.14
3:A:599:HOH:O	3:B:581:HOH:O[1_565]	2.09	0.11
3:B:489:HOH:O	3:B:664:HOH:O[1_565]	2.13	0.07
3:B:523:HOH:O	3:B:528:HOH:O[2_556]	2.14	0.06
3:A:500:HOH:O	3:A:528:HOH:O[2_647]	2.16	0.04

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	372/393 (95%)	364 (98%)	7 (2%)	1 (0%)	46	29
1	B	372/393 (95%)	357 (96%)	15 (4%)	0	100	100
All	All	744/786 (95%)	721 (97%)	22 (3%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ALA

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	312/323 (97%)	308 (99%)	4 (1%)	76	68
1	B	312/323 (97%)	304 (97%)	8 (3%)	54	37
All	All	624/646 (97%)	612 (98%)	12 (2%)	65	52

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	136	ASN
1	A	144	TYR
1	A	263	HIS
1	B	76	LYS

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Mol	Chain	Res	Type
1	B	118	LEU
1	B	125	ASP
1	B	144	TYR
1	B	263	HIS
1	B	274	LYS
1	B	286	LYS
1	B	344	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	185	HIS
1	A	216	HIS
1	A	234	ASN
1	A	263	HIS
1	B	126	HIS
1	B	185	HIS
1	B	216	HIS
1	B	263	HIS

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](#)

2 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	SO4	A	401	-	4,4,4	1.24	0	6,6,6	1.53	2 (33%)
2	SO4	B	402	-	4,4,4	1.51	1 (25%)	6,6,6	1.38	2 (33%)

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	SO4	A	401	-	-	0/0/0/0	0/0/0/0
2	SO4	B	402	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	SO4	O3-S	2.12	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SO4	O2-S-O1	-2.52	101.50	109.50
2	B	402	SO4	O2-S-O1	-2.26	102.34	109.50
2	A	401	SO4	O4-S-O3	-2.08	100.51	108.98
2	B	402	SO4	O4-S-O1	2.12	129.95	110.19

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	B	402	SO4	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 [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	374/393 (95%)	-0.84	0	100 100	6, 15, 39, 69	0
1	B	374/393 (95%)	-0.56	4 (1%)	82 80	5, 16, 55, 85	0
All	All	748/786 (95%)	-0.70	4 (0%)	91 90	5, 15, 48, 85	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	374	ALA	4.1
1	B	133	ILE	2.4
1	B	260	GLU	2.3
1	B	372	ALA	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. 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(\AA^2)	Q<0.9
2	SO4	B	402	5/5	0.89	0.14	26.63	37,39,48,52	0
2	SO4	A	401	5/5	0.93	0.12	5.64	40,43,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.