



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:25 AM GMT

PDB ID : 2Q2Q
Title : Structure of D-3-Hydroxybutyrate Dehydrogenase from Pseudomonas putida
Authors : Paithankar, K.S.; Feller, C.; Kuettner, E.B.; Keim, A.; Grunow, M.; Strater, N.
Deposited on : 2007-05-29
Resolution : 2.02 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

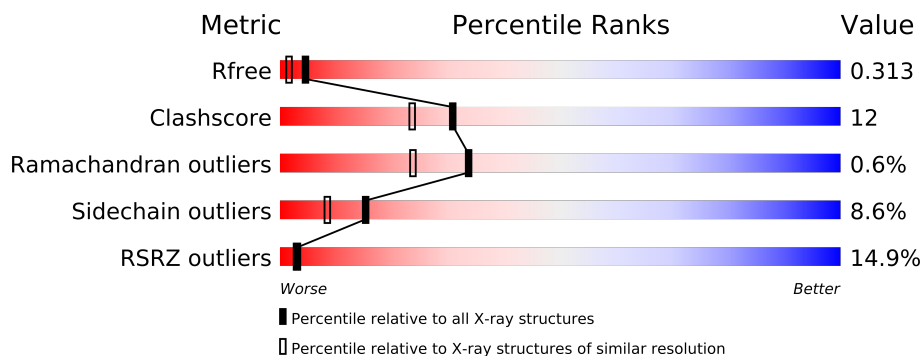
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.02 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}	66092	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	255	
1	B	255	
1	C	255	
1	D	255	
1	E	255	
1	F	255	
1	G	255	
1	H	255	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15261 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Beta-D-hydroxybutyrate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1843	1171	330	338	4			
1	B	252	Total	C	N	O	S	0	0	0
			1852	1176	332	340	4			
1	C	243	Total	C	N	O	S	0	0	0
			1784	1137	319	324	4			
1	D	255	Total	C	N	O	S	0	0	0
			1869	1185	336	344	4			
1	E	249	Total	C	N	O	S	0	0	0
			1833	1165	329	335	4			
1	F	238	Total	C	N	O	S	0	0	0
			1742	1110	311	317	4			
1	G	251	Total	C	N	O	S	0	0	0
			1845	1173	331	337	4			
1	H	240	Total	C	N	O	S	0	0	0
			1758	1120	314	320	4			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	83	Total	O	0	0
			83	83		
3	C	37	Total	O	0	0
			37	37		
3	D	70	Total	O	0	0
			70	70		
3	E	55	Total	O	0	0
			55	55		
3	F	50	Total	O	0	0
			50	50		

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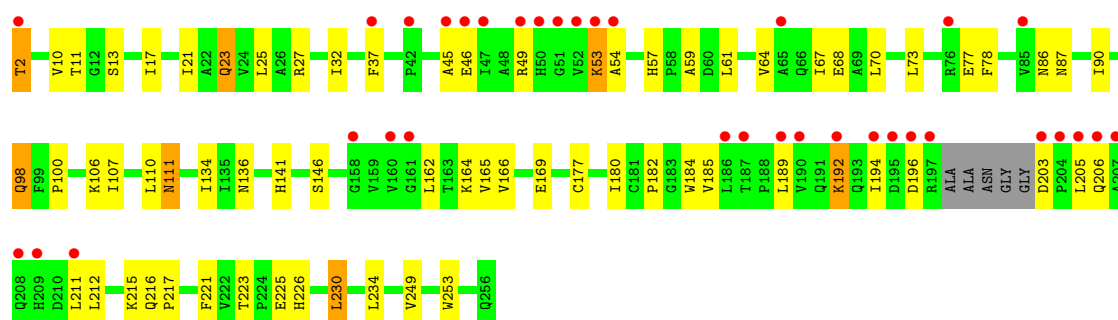
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	71	Total	O	0	0
			71	71		
3	H	44	Total	O	0	0
			44	44		

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.

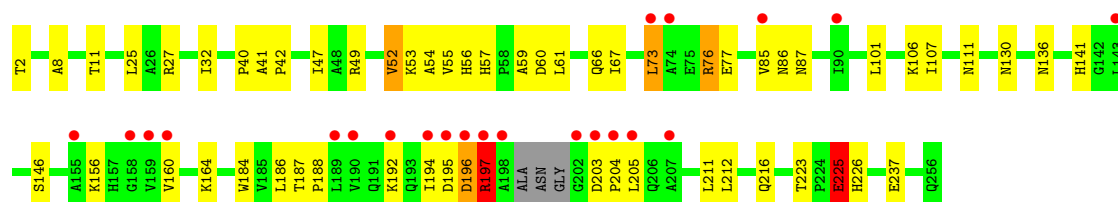
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain A: 



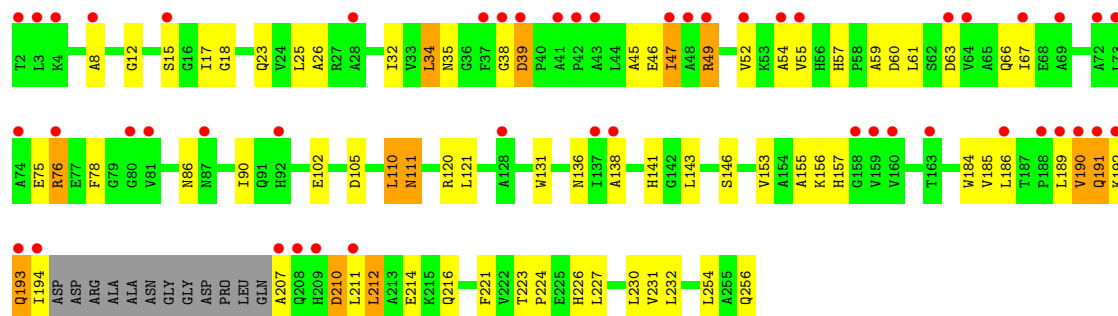
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain B: 



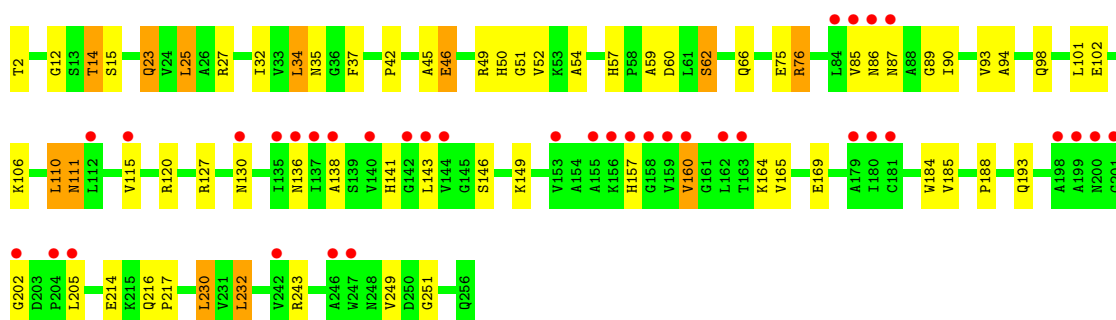
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain C: 



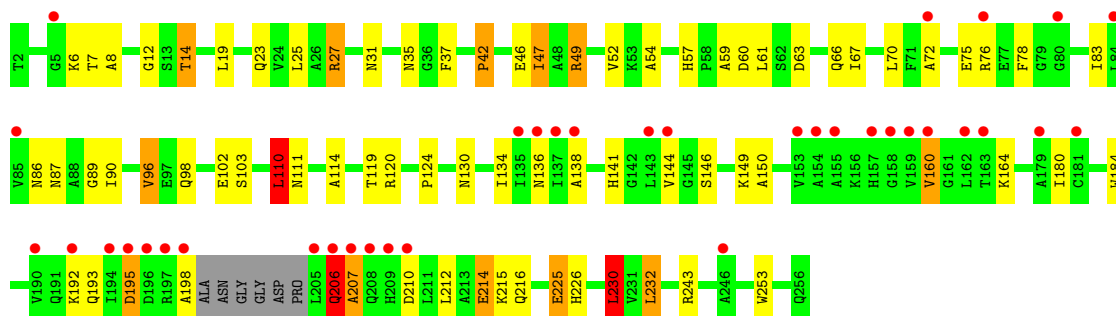
- Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain D: 



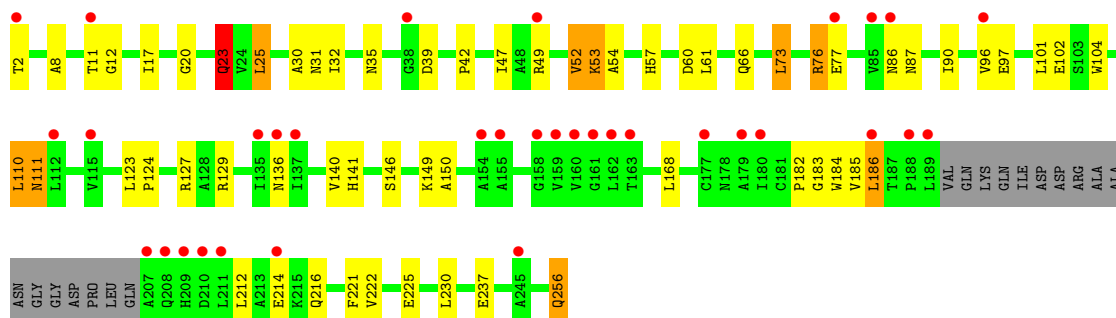
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain E:



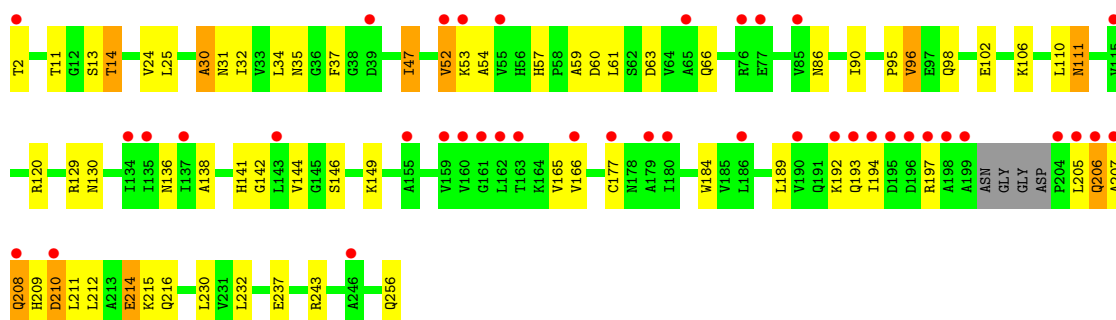
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain F:



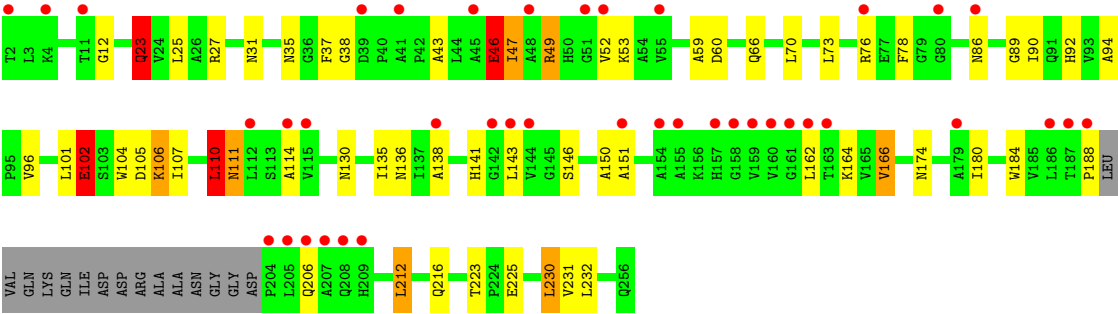
• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain G:



• Molecule 1: Beta-D-hydroxybutyrate dehydrogenase

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.46Å 59.91Å 116.52Å 90.00° 113.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 29.96 – 2.02	Depositor EDS
% Data completeness (in resolution range)	96.4 (30.00-2.02) 96.4 (29.96-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.274 0.253 , 0.313	Depositor DCC
R_{free} test set	5242 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.6	EDS
Estimated twinning fraction	0.009 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 104909 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15261	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 44.55 % 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 1.5024e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	1.20	4/1879 (0.2%)	0.99	1/2560 (0.0%)
1	B	1.20	5/1888 (0.3%)	1.04	5/2572 (0.2%)
1	C	1.06	2/1819 (0.1%)	1.00	2/2478 (0.1%)
1	D	1.39	12/1906 (0.6%)	1.16	15/2598 (0.6%)
1	E	1.37	8/1868 (0.4%)	1.18	11/2544 (0.4%)
1	F	1.33	8/1777 (0.5%)	1.05	5/2422 (0.2%)
1	G	1.33	14/1881 (0.7%)	1.13	10/2562 (0.4%)
1	H	1.32	8/1794 (0.4%)	1.11	7/2445 (0.3%)
All	All	1.28	61/14812 (0.4%)	1.08	56/20181 (0.3%)

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	E	0	2
1	H	0	2
All	All	0	4

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	206	GLN	CD-OE1	15.60	1.58	1.24
1	G	209	HIS	CE1-NE2	14.02	1.65	1.32
1	E	206	GLN	CD-NE2	13.54	1.66	1.32
1	D	75	GLU	CG-CD	12.25	1.70	1.51
1	G	209	HIS	CG-ND1	10.21	1.61	1.38
1	D	214	GLU	CG-CD	9.54	1.66	1.51
1	F	214	GLU	CB-CG	8.57	1.68	1.52
1	F	102	GLU	CB-CG	8.56	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	23	GLN	CG-CD	8.55	1.70	1.51
1	D	115	VAL	CB-CG1	8.27	1.70	1.52
1	G	209	HIS	CG-CD2	7.61	1.48	1.35
1	F	102	GLU	CG-CD	7.44	1.63	1.51
1	F	104	TRP	CB-CG	7.31	1.63	1.50
1	D	75	GLU	CB-CG	7.25	1.66	1.52
1	D	46	GLU	CD-OE2	7.23	1.33	1.25
1	H	102	GLU	CG-CD	7.09	1.62	1.51
1	E	225	GLU	CG-CD	7.08	1.62	1.51
1	D	185	VAL	CB-CG1	6.99	1.67	1.52
1	E	160	VAL	CB-CG2	6.90	1.67	1.52
1	D	62	SER	CB-OG	-6.81	1.33	1.42
1	F	256	GLN	C-OXT	6.75	1.36	1.23
1	G	30	ALA	CA-CB	6.59	1.66	1.52
1	E	144	VAL	CB-CG2	6.59	1.66	1.52
1	G	237	GLU	CG-CD	6.52	1.61	1.51
1	B	85	VAL	CB-CG1	6.32	1.66	1.52
1	A	225	GLU	CG-CD	6.30	1.61	1.51
1	H	102	GLU	CB-CG	6.21	1.64	1.52
1	B	237	GLU	CG-CD	6.12	1.61	1.51
1	D	23	GLN	CG-CD	5.95	1.64	1.51
1	H	188	PRO	C-O	5.83	1.34	1.23
1	G	177	CYS	CB-SG	-5.74	1.72	1.81
1	H	94	ALA	CA-CB	5.67	1.64	1.52
1	F	23	GLN	CG-CD	5.64	1.64	1.51
1	E	102	GLU	CG-CD	5.63	1.60	1.51
1	C	155	ALA	CA-CB	5.61	1.64	1.52
1	G	102	GLU	CG-CD	5.61	1.60	1.51
1	A	225	GLU	CB-CG	5.60	1.62	1.52
1	E	214	GLU	CD-OE1	5.59	1.31	1.25
1	F	53	LYS	CE-NZ	5.57	1.62	1.49
1	E	96	VAL	CB-CG2	-5.54	1.41	1.52
1	B	160	VAL	CB-CG2	5.52	1.64	1.52
1	D	249	VAL	CB-CG1	5.50	1.64	1.52
1	A	98	GLN	CB-CG	-5.47	1.37	1.52
1	B	2	THR	CB-CG2	5.47	1.70	1.52
1	H	23	GLN	CB-CG	5.46	1.67	1.52
1	B	225	GLU	CG-CD	5.46	1.60	1.51
1	A	2	THR	CA-CB	5.42	1.67	1.53
1	D	76	ARG	CG-CD	5.39	1.65	1.51
1	H	166	VAL	CB-CG2	5.37	1.64	1.52
1	G	130	ASN	CB-CG	5.35	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	144	VAL	CB-CG1	5.32	1.64	1.52
1	D	160	VAL	CB-CG1	5.30	1.64	1.52
1	G	165	VAL	CA-CB	5.27	1.65	1.54
1	H	164	LYS	CD-CE	5.24	1.64	1.51
1	F	149	LYS	CD-CE	5.23	1.64	1.51
1	G	142	GLY	N-CA	5.22	1.53	1.46
1	G	166	VAL	CB-CG2	5.22	1.63	1.52
1	C	46	GLU	C-O	5.20	1.33	1.23
1	D	85	VAL	CB-CG2	5.10	1.63	1.52
1	G	96	VAL	CB-CG1	-5.06	1.42	1.52
1	G	24	VAL	CB-CG2	5.01	1.63	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	243	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	E	243	ARG	NE-CZ-NH1	12.62	126.61	120.30
1	G	129	ARG	NE-CZ-NH2	-9.81	115.40	120.30
1	C	63	ASP	CB-CG-OD2	8.27	125.74	118.30
1	E	63	ASP	CB-CG-OD1	7.68	125.21	118.30
1	D	120	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	D	230	LEU	CB-CG-CD2	7.30	123.41	111.00
1	D	62	SER	CB-CA-C	-7.24	96.34	110.10
1	A	98	GLN	CB-CA-C	-7.20	96.01	110.40
1	D	243	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	E	230	LEU	CB-CG-CD2	7.13	123.12	111.00
1	E	195	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	H	106	LYS	CD-CE-NZ	7.02	127.85	111.70
1	D	143	LEU	CA-CB-CG	-6.94	99.34	115.30
1	H	212	LEU	CA-CB-CG	6.88	131.13	115.30
1	D	120	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	F	256	GLN	CA-C-O	-6.75	105.93	120.10
1	H	143	LEU	CB-CG-CD1	6.71	122.40	111.00
1	D	127	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	49	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	34	LEU	CA-CB-CG	6.66	130.61	115.30
1	D	76	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	F	127	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	96	VAL	CB-CA-C	-6.61	98.85	111.40
1	E	96	VAL	CG1-CB-CG2	-6.47	100.55	110.90
1	F	183	GLY	N-CA-C	-6.44	96.99	113.10
1	G	205	LEU	CA-CB-CG	6.27	129.73	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	120	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	E	243	ARG	CG-CD-NE	-6.07	99.05	111.80
1	B	49	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	H	110	LEU	CB-CG-CD2	5.92	121.06	111.00
1	D	34	LEU	CB-CG-CD1	5.91	121.05	111.00
1	E	110	LEU	CB-CG-CD2	5.87	120.97	111.00
1	D	243	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	E	195	ASP	CB-CG-OD1	5.81	123.53	118.30
1	G	129	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	25	LEU	CB-CG-CD1	5.72	120.72	111.00
1	E	232	LEU	CA-CB-CG	5.68	128.37	115.30
1	H	105	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	120	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	75	GLU	CA-CB-CG	5.50	125.49	113.40
1	B	76	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	G	243	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	243	ARG	CD-NE-CZ	5.41	131.18	123.60
1	D	232	LEU	CB-CG-CD2	5.38	120.14	111.00
1	B	27	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	F	129	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	C	105	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	52	VAL	CG1-CB-CG2	5.24	119.29	110.90
1	F	168	LEU	CB-CG-CD2	-5.23	102.11	111.00
1	H	232	LEU	CB-CG-CD2	-5.21	102.13	111.00
1	G	63	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	52	VAL	CG1-CB-CG2	5.20	119.23	110.90
1	G	189	LEU	CB-CG-CD2	-5.19	102.17	111.00
1	H	70	LEU	CA-CB-CG	5.17	127.19	115.30
1	G	210	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	206	GLN	Sidechain
1	E	207	ALA	Peptide
1	H	38	GLY	Peptide
1	H	49	ARG	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1843	0	1865	57	0
1	B	1852	0	1873	35	0
1	C	1784	0	1814	56	0
1	D	1869	0	1888	43	0
1	E	1833	0	1859	51	0
1	F	1742	0	1765	46	0
1	G	1845	0	1872	33	0
1	H	1758	0	1781	38	0
2	C	44	0	26	1	0
2	D	44	0	26	2	0
2	E	44	0	26	4	0
2	F	44	0	26	3	0
2	G	44	0	26	2	0
2	H	44	0	26	1	0
3	A	61	0	0	2	0
3	B	83	0	0	2	0
3	C	37	0	0	1	0
3	D	70	0	0	4	0
3	E	55	0	0	1	1
3	F	50	0	0	1	0
3	G	71	0	0	1	1
3	H	44	0	0	2	0
All	All	15261	0	14873	350	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (350) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:32:ILE:HG22	1:C:34:LEU:HD13	1.27	1.08
1:F:186:LEU:HD23	1:F:186:LEU:H	1.19	1.07
1:C:32:ILE:HG22	1:C:34:LEU:CD1	1.90	1.01
1:E:184:TRP:H	1:E:216:GLN:HE22	1.09	1.00
1:C:32:ILE:CG2	1:C:34:LEU:CD1	2.39	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:184:TRP:H	1:F:216:GLN:HE22	1.08	0.98
1:F:141:HIS:HE1	1:F:146:SER:OG	1.49	0.94
1:H:184:TRP:H	1:H:216:GLN:HE22	1.10	0.94
1:D:14:THR:HG21	1:D:37:PHE:O	1.68	0.92
1:F:186:LEU:H	1:F:186:LEU:CD2	1.83	0.90
1:C:32:ILE:CG2	1:C:34:LEU:HD13	2.03	0.87
1:D:42:PRO:O	1:D:46:GLU:HG2	1.74	0.87
1:F:256:GLN:OXT	3:F:317:HOH:O	1.93	0.87
1:H:96:VAL:HG12	1:H:150:ALA:HB2	1.57	0.87
1:A:184:TRP:H	1:A:216:GLN:HE22	1.17	0.87
1:C:184:TRP:H	1:C:216:GLN:HE22	1.23	0.86
1:G:184:TRP:H	1:G:216:GLN:HE22	1.24	0.86
1:E:27:ARG:NH1	3:E:342:HOH:O	2.09	0.86
1:B:184:TRP:H	1:B:216:GLN:HE22	1.25	0.84
1:G:141:HIS:HE1	1:G:146:SER:OG	1.62	0.83
1:A:189:LEU:O	1:A:189:LEU:HD12	1.79	0.83
1:G:14:THR:HG21	1:G:37:PHE:O	1.77	0.82
1:C:45:ALA:O	1:C:49:ARG:HG2	1.80	0.81
1:A:57:HIS:CE1	1:A:59:ALA:HB2	2.15	0.81
1:D:184:TRP:H	1:D:216:GLN:HE22	1.27	0.80
1:C:32:ILE:HG21	1:C:34:LEU:CD1	2.12	0.80
1:D:51:GLY:HA2	1:F:53:LYS:HD3	1.65	0.79
1:G:57:HIS:HD2	1:G:59:ALA:H	1.31	0.79
1:E:86:ASN:HD22	1:E:136:ASN:HD21	1.32	0.78
3:D:365:HOH:O	1:H:92:HIS:HD2	1.65	0.78
1:E:90:ILE:H	1:E:111:ASN:HD21	1.33	0.77
1:C:32:ILE:HG21	1:C:34:LEU:HD11	1.68	0.76
1:G:95:PRO:HG2	1:G:98:GLN:OE1	1.86	0.75
1:A:53:LYS:HG3	1:A:78:PHE:HE1	1.52	0.75
1:E:14:THR:HG22	2:E:300:NAD:O3B	1.87	0.74
1:H:90:ILE:H	1:H:111:ASN:HD21	1.33	0.74
1:A:111:ASN:HD22	1:A:111:ASN:N	1.83	0.74
1:E:184:TRP:N	1:E:216:GLN:HE22	1.85	0.74
1:F:141:HIS:CE1	1:F:146:SER:OG	2.38	0.74
1:B:86:ASN:HD22	1:B:136:ASN:HD21	1.34	0.74
1:C:76:ARG:HA	1:C:76:ARG:NE	2.03	0.73
1:B:86:ASN:HD22	1:B:136:ASN:ND2	1.85	0.73
1:F:90:ILE:H	1:F:111:ASN:HD21	1.34	0.73
1:E:72:ALA:O	1:E:76:ARG:HG3	1.88	0.73
1:G:57:HIS:CD2	1:G:59:ALA:H	2.06	0.72
1:G:47:ILE:HD11	1:G:54:ALA:HB2	1.70	0.72
1:B:57:HIS:HB2	1:B:73:LEU:HD12	1.70	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:101:LEU:HD12	1:B:101:LEU:H	1.54	0.71
1:F:186:LEU:HD23	1:F:186:LEU:N	1.99	0.71
1:C:38:GLY:O	1:C:39:ASP:CB	2.38	0.71
1:G:86:ASN:HD22	1:G:136:ASN:ND2	1.88	0.71
1:D:90:ILE:H	1:D:111:ASN:HD21	1.38	0.70
1:A:184:TRP:H	1:A:216:GLN:NE2	1.90	0.69
1:E:14:THR:HG21	1:E:37:PHE:O	1.91	0.69
1:A:86:ASN:HD22	1:A:136:ASN:ND2	1.91	0.69
1:E:96:VAL:HG22	1:E:150:ALA:HB2	1.74	0.69
1:A:57:HIS:HB2	1:A:73:LEU:HD23	1.73	0.69
1:A:141:HIS:HE1	1:A:146:SER:OG	1.76	0.69
1:G:90:ILE:H	1:G:111:ASN:HD21	1.42	0.68
1:F:73:LEU:HD22	1:F:77:GLU:HG2	1.75	0.68
1:B:164:LYS:NZ	1:C:157:HIS:HE1	1.92	0.68
1:C:111:ASN:HD22	1:C:111:ASN:N	1.91	0.68
1:F:30:ALA:O	1:F:52:VAL:HG11	1.94	0.67
1:F:184:TRP:N	1:F:216:GLN:HE22	1.87	0.67
1:H:90:ILE:HG13	1:H:107:ILE:CD1	2.25	0.67
1:E:86:ASN:HD22	1:E:136:ASN:ND2	1.93	0.67
1:H:184:TRP:N	1:H:216:GLN:HE22	1.90	0.66
1:D:12:GLY:H	1:D:35:ASN:HD22	1.42	0.66
1:G:86:ASN:HD22	1:G:136:ASN:HD21	1.42	0.66
1:C:60:ASP:H	1:C:66:GLN:NE2	1.93	0.65
1:F:47:ILE:CG2	1:F:54:ALA:HB2	2.25	0.65
1:F:186:LEU:HD22	1:F:221:PHE:HB3	1.78	0.65
1:C:57:HIS:HD2	1:C:59:ALA:H	1.45	0.65
1:H:60:ASP:H	1:H:66:GLN:NE2	1.95	0.65
3:D:365:HOH:O	1:H:92:HIS:CD2	2.46	0.64
1:B:55:VAL:HG11	1:B:77:GLU:HG3	1.79	0.64
1:E:49:ARG:C	1:E:49:ARG:HD3	2.17	0.64
1:F:184:TRP:H	1:F:216:GLN:NE2	1.89	0.63
1:D:138:ALA:O	2:D:300:NAD:H6N	1.98	0.63
1:E:47:ILE:CG1	1:E:54:ALA:HB2	2.28	0.63
1:H:141:HIS:HE1	1:H:146:SER:OG	1.80	0.63
1:E:184:TRP:H	1:E:216:GLN:NE2	1.88	0.63
1:A:90:ILE:HG22	1:A:111:ASN:HD21	1.63	0.62
1:C:184:TRP:N	1:C:216:GLN:HE22	1.93	0.62
1:E:47:ILE:HD11	1:E:54:ALA:HB2	1.79	0.62
1:H:73:LEU:HD12	1:H:76:ARG:NH2	2.15	0.62
1:D:45:ALA:O	1:D:49:ARG:HD2	1.99	0.62
1:C:143:LEU:HD12	1:C:254:LEU:CD1	2.29	0.62
1:G:256:GLN:OXT	3:G:310:HOH:O	2.16	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:90:ILE:HB	1:A:110:LEU:HD23	1.82	0.61
1:D:51:GLY:HA2	1:F:53:LYS:CD	2.29	0.61
1:H:102:GLU:O	1:H:106:LYS:HE3	2.01	0.61
1:A:86:ASN:HD22	1:A:136:ASN:HD21	1.47	0.61
1:C:61:LEU:HD22	1:C:67:ILE:HG12	1.83	0.61
1:F:47:ILE:HG22	1:F:54:ALA:HB2	1.81	0.60
1:H:86:ASN:HD22	1:H:136:ASN:HD21	1.50	0.60
1:D:141:HIS:HE1	1:D:146:SER:OG	1.83	0.60
1:E:138:ALA:O	2:E:300:NAD:H6N	2.02	0.60
1:D:57:HIS:CD2	1:D:59:ALA:HB2	2.36	0.60
1:A:164:LYS:NZ	1:D:157:HIS:HE1	2.00	0.60
1:D:60:ASP:OD1	1:D:62:SER:HB2	2.02	0.60
1:H:92:HIS:HE1	3:H:338:HOH:O	1.83	0.59
1:A:180:ILE:HG12	1:A:230:LEU:HD13	1.84	0.59
1:G:47:ILE:CD1	1:G:52:VAL:HG12	2.33	0.59
1:H:102:GLU:C	1:H:106:LYS:HE3	2.23	0.59
1:A:184:TRP:N	1:A:216:GLN:HE22	1.95	0.59
1:F:31:ASN:HA	1:F:52:VAL:HG13	1.85	0.59
1:C:110:LEU:HB3	1:C:111:ASN:HD22	1.68	0.59
1:H:184:TRP:H	1:H:216:GLN:NE2	1.92	0.58
1:D:98:GLN:HA	1:D:98:GLN:HE21	1.66	0.58
1:C:47:ILE:HG22	1:C:54:ALA:HB2	1.84	0.58
1:B:61:LEU:O	1:B:67:ILE:HD11	2.04	0.58
1:C:38:GLY:O	1:C:39:ASP:HB3	2.03	0.58
1:D:98:GLN:HA	1:D:98:GLN:NE2	2.19	0.58
1:E:86:ASN:HB2	1:E:136:ASN:HD22	1.67	0.58
1:A:37:PHE:HB2	3:A:315:HOH:O	2.03	0.58
1:D:149:LYS:NZ	1:D:193:GLN:HE22	2.02	0.58
1:E:31:ASN:OD1	1:E:52:VAL:HG22	2.04	0.58
1:H:86:ASN:HD22	1:H:136:ASN:ND2	2.00	0.57
1:F:12:GLY:H	1:F:35:ASN:HD22	1.52	0.57
1:H:31:ASN:HA	1:H:52:VAL:HG13	1.86	0.57
1:G:206:GLN:OE1	1:G:206:GLN:HA	2.04	0.57
1:H:225:GLU:CD	1:H:225:GLU:H	2.08	0.57
1:B:184:TRP:N	1:B:216:GLN:HE22	1.97	0.57
1:B:141:HIS:HE1	1:B:146:SER:OG	1.87	0.57
1:H:12:GLY:H	1:H:35:ASN:HD22	1.51	0.57
1:D:98:GLN:CA	1:D:98:GLN:NE2	2.67	0.56
1:E:8:ALA:HA	1:E:83:ILE:O	2.05	0.56
1:H:46:GLU:O	1:H:49:ARG:HG3	2.05	0.56
1:E:149:LYS:NZ	1:E:193:GLN:HE22	2.03	0.56
1:B:60:ASP:H	1:B:66:GLN:NE2	2.03	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:86:ASN:HD22	1:D:136:ASN:ND2	2.03	0.56
1:F:35:ASN:HD21	2:F:300:NAD:H2A	1.71	0.56
1:C:8:ALA:HB3	1:C:32:ILE:HD13	1.88	0.55
1:E:110:LEU:HB3	1:E:111:ASN:HD22	1.70	0.55
1:H:180:ILE:HG12	1:H:230:LEU:HD13	1.88	0.55
1:E:89:GLY:HA2	1:E:110:LEU:HD13	1.88	0.55
1:C:143:LEU:HD12	1:C:254:LEU:HD13	1.89	0.55
1:A:46:GLU:OE2	1:A:49:ARG:NH1	2.40	0.55
1:C:17:ILE:HD11	1:C:185:VAL:HG21	1.88	0.55
1:G:214:GLU:HB3	1:G:215:LYS:HG2	1.89	0.55
1:C:12:GLY:H	1:C:35:ASN:HD22	1.55	0.54
1:F:17:ILE:HD11	1:F:185:VAL:HG21	1.88	0.54
1:A:45:ALA:O	1:A:49:ARG:HG2	2.08	0.54
1:D:57:HIS:HD2	1:D:59:ALA:H	1.56	0.54
1:B:225:GLU:CD	1:B:225:GLU:H	2.10	0.54
1:H:43:ALA:O	1:H:47:ILE:HG12	2.08	0.54
1:A:100:PRO:HB3	1:H:37:PHE:CD2	2.43	0.53
1:D:111:ASN:N	1:D:111:ASN:HD22	2.07	0.53
1:B:164:LYS:HZ1	1:C:157:HIS:HE1	1.55	0.53
1:A:90:ILE:HG23	1:A:107:ILE:HG12	1.90	0.53
1:E:47:ILE:CD1	1:E:54:ALA:HB2	2.39	0.53
1:B:184:TRP:H	1:B:216:GLN:NE2	2.02	0.53
1:E:207:ALA:O	1:E:210:ASP:HB2	2.09	0.53
1:A:53:LYS:HG3	1:A:78:PHE:CE1	2.38	0.53
1:H:89:GLY:HA2	1:H:110:LEU:HD13	1.91	0.52
1:C:141:HIS:HE1	1:C:146:SER:OG	1.92	0.52
1:A:23:GLN:NE2	1:A:46:GLU:HG3	2.24	0.52
1:H:223:THR:HB	1:H:225:GLU:OE1	2.09	0.52
1:C:184:TRP:H	1:C:216:GLN:NE2	2.00	0.52
1:E:42:PRO:O	1:E:46:GLU:HG2	2.09	0.52
1:A:111:ASN:N	1:A:111:ASN:ND2	2.56	0.52
1:C:138:ALA:HA	1:C:156:LYS:HD2	1.92	0.51
1:E:206:GLN:CD	1:E:206:GLN:C	2.69	0.51
1:C:256:GLN:O	3:C:332:HOH:O	2.19	0.51
1:C:184:TRP:CD1	1:C:212:LEU:HD12	2.45	0.51
1:D:86:ASN:HD22	1:D:136:ASN:HD21	1.57	0.51
1:C:26:ALA:HB2	1:C:32:ILE:HG13	1.93	0.51
1:H:135:ILE:HD12	1:H:231:VAL:HG13	1.92	0.51
1:A:184:TRP:CZ3	1:A:211:LEU:HD21	2.46	0.51
1:A:57:HIS:HB3	1:A:70:LEU:HD13	1.92	0.51
1:F:90:ILE:HG12	1:F:110:LEU:HD12	1.93	0.51
1:B:107:ILE:HG23	1:B:111:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:53:LYS:HG2	1:H:78:PHE:CE2	2.46	0.51
1:D:98:GLN:CA	1:D:98:GLN:HE21	2.24	0.50
1:C:17:ILE:HA	1:C:224:PRO:HB3	1.92	0.50
1:F:47:ILE:HG21	1:F:54:ALA:HB2	1.92	0.50
1:A:61:LEU:O	1:A:67:ILE:HD11	2.12	0.50
1:E:141:HIS:HE1	1:E:146:SER:OG	1.94	0.50
1:G:11:THR:HB	1:G:61:LEU:HD11	1.93	0.50
1:D:165:VAL:O	1:D:169:GLU:HG3	2.11	0.50
1:E:19:LEU:O	1:E:23:GLN:HG3	2.12	0.49
1:D:184:TRP:H	1:D:216:GLN:NE2	2.03	0.49
1:A:141:HIS:CE1	1:A:146:SER:OG	2.62	0.49
1:H:73:LEU:HD12	1:H:76:ARG:HH21	1.75	0.49
1:C:138:ALA:O	2:C:300:NAD:H6N	2.12	0.49
1:C:191:GLN:HA	1:C:194:ILE:CD1	2.42	0.49
1:D:32:ILE:O	1:D:54:ALA:HA	2.12	0.49
1:A:23:GLN:NE2	1:A:46:GLU:O	2.45	0.49
1:E:207:ALA:HA	1:E:210:ASP:OD1	2.12	0.49
1:C:55:VAL:CG2	1:C:78:PHE:HE2	2.25	0.49
1:C:141:HIS:HB3	1:C:153:VAL:HG22	1.94	0.49
1:E:57:HIS:CD2	1:E:59:ALA:HB2	2.48	0.49
1:A:64:VAL:O	1:A:68:GLU:HG3	2.13	0.49
1:C:207:ALA:O	1:C:210:ASP:HB2	2.12	0.49
1:G:184:TRP:N	1:G:216:GLN:HE22	2.02	0.49
1:G:14:THR:HG22	2:G:300:NAD:O3B	2.13	0.49
1:E:87:ASN:O	2:E:300:NAD:H4D	2.13	0.49
1:D:86:ASN:HB2	1:D:136:ASN:HD22	1.77	0.48
1:D:27:ARG:HG3	1:D:50:HIS:CE1	2.48	0.48
1:B:40:PRO:HB3	1:B:56:HIS:CG	2.48	0.48
1:E:195:ASP:O	1:E:198:ALA:HB3	2.13	0.48
1:A:194:ILE:HD11	1:A:221:PHE:CZ	2.49	0.48
1:A:73:LEU:HD12	1:A:77:GLU:CG	2.43	0.48
1:A:57:HIS:HB2	1:A:73:LEU:CD2	2.43	0.48
1:E:214:GLU:HG3	1:E:215:LYS:HG2	1.96	0.48
1:E:31:ASN:OD1	1:E:52:VAL:CG2	2.62	0.48
1:G:57:HIS:CD2	1:G:59:ALA:HB2	2.49	0.48
1:A:192:LYS:O	1:A:196:ASP:OD2	2.32	0.48
1:C:191:GLN:HA	1:C:194:ILE:HD12	1.95	0.47
1:B:41:ALA:HB3	1:B:42:PRO:HD3	1.96	0.47
1:A:73:LEU:HD12	1:A:77:GLU:HG2	1.94	0.47
1:A:57:HIS:HE1	1:A:59:ALA:HB2	1.71	0.47
1:D:57:HIS:CD2	1:D:59:ALA:H	2.33	0.47
1:G:30:ALA:O	1:G:52:VAL:HG11	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:20:GLY:O	1:F:23:GLN:NE2	2.47	0.47
1:C:75:GLU:OE1	1:C:76:ARG:NH1	2.47	0.47
1:G:86:ASN:HB2	1:G:136:ASN:HD22	1.80	0.47
1:D:46:GLU:OE2	1:D:49:ARG:NH1	2.47	0.47
1:C:184:TRP:HD1	1:C:212:LEU:HD12	1.79	0.47
1:F:73:LEU:HD23	1:F:76:ARG:NH2	2.29	0.47
1:F:185:VAL:HG13	1:F:222:VAL:O	2.15	0.47
1:G:194:ILE:HG21	1:G:208:GLN:HB3	1.95	0.47
1:F:39:ASP:O	1:F:42:PRO:HD2	2.13	0.47
1:F:11:THR:HB	1:F:61:LEU:HD11	1.97	0.47
1:D:160:VAL:HG12	1:D:164:LYS:HE3	1.96	0.47
1:F:86:ASN:HD22	1:F:136:ASN:ND2	2.11	0.47
1:B:223:THR:H	1:B:226:HIS:CD2	2.33	0.47
1:C:111:ASN:N	1:C:111:ASN:ND2	2.62	0.47
1:C:12:GLY:O	1:C:18:GLY:HA3	2.15	0.47
1:A:86:ASN:HB2	1:A:136:ASN:HD22	1.80	0.46
1:D:87:ASN:O	2:D:300:NAD:H4D	2.16	0.46
1:E:226:HIS:HE1	1:F:237:GLU:OE1	1.98	0.46
1:A:32:ILE:O	1:A:54:ALA:HA	2.15	0.46
1:H:130:ASN:O	1:H:174:ASN:HB2	2.15	0.46
1:G:197:ARG:NH2	1:G:214:GLU:OE2	2.42	0.46
1:G:149:LYS:NZ	1:G:193:GLN:HE22	2.13	0.46
1:A:215:LYS:HB3	1:A:253:TRP:CE2	2.50	0.46
1:G:61:LEU:HG	2:G:300:NAD:H2A	1.98	0.46
1:G:47:ILE:CD1	1:G:54:ALA:HB2	2.44	0.46
1:C:190:VAL:O	1:C:193:GLN:N	2.49	0.46
1:C:227:LEU:O	1:C:231:VAL:HG23	2.14	0.46
1:E:47:ILE:CD1	1:E:52:VAL:HG13	2.46	0.46
1:A:192:LYS:HE3	1:A:192:LYS:N	2.30	0.46
1:A:17:ILE:HG22	1:A:21:ILE:HD12	1.97	0.46
1:A:90:ILE:HG22	1:A:111:ASN:ND2	2.30	0.46
1:F:87:ASN:O	2:F:300:NAD:H4D	2.16	0.46
1:A:141:HIS:HD2	3:A:316:HOH:O	1.99	0.46
1:D:57:HIS:HD2	1:D:59:ALA:HB2	1.79	0.45
1:F:60:ASP:H	1:F:66:GLN:NE2	2.14	0.45
1:E:57:HIS:HD2	1:E:59:ALA:H	1.63	0.45
1:A:17:ILE:HG12	1:A:185:VAL:HG11	1.99	0.45
1:A:90:ILE:H	1:A:111:ASN:HD21	1.63	0.45
1:C:143:LEU:CD1	1:C:254:LEU:HD13	2.46	0.45
1:F:96:VAL:HG12	1:F:150:ALA:HB2	1.99	0.45
1:C:86:ASN:HD22	1:C:136:ASN:ND2	2.14	0.45
1:G:31:ASN:OD1	1:G:53:LYS:HB2	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:162:LEU:O	1:H:166:VAL:HG23	2.17	0.45
1:A:73:LEU:CD1	1:A:77:GLU:HG3	2.46	0.45
1:E:61:LEU:HG	2:E:300:NAD:H2A	1.99	0.45
1:B:101:LEU:HD21	1:C:120:ARG:CZ	2.47	0.45
1:B:156:LYS:NZ	3:B:334:HOH:O	2.39	0.45
1:A:134:ILE:O	1:A:177:CYS:HA	2.16	0.45
1:E:60:ASP:H	1:E:66:GLN:NE2	2.15	0.45
1:E:49:ARG:C	1:E:49:ARG:CD	2.85	0.45
1:E:180:ILE:HG12	1:E:230:LEU:HD13	1.98	0.45
1:A:203:ASP:HB3	1:A:206:GLN:HB3	1.99	0.45
1:E:206:GLN:CD	1:E:207:ALA:N	2.70	0.44
1:F:86:ASN:HB2	1:F:136:ASN:HD22	1.82	0.44
1:F:73:LEU:HD23	1:F:76:ARG:HH21	1.82	0.44
1:B:61:LEU:HD22	1:B:67:ILE:HG12	1.99	0.44
1:D:27:ARG:CG	1:D:50:HIS:CE1	3.00	0.44
1:B:211:LEU:HA	1:B:211:LEU:HD12	1.83	0.44
1:D:184:TRP:N	1:D:216:GLN:HE22	2.05	0.44
1:B:187:THR:HB	1:B:188:PRO:CD	2.47	0.44
1:E:57:HIS:HB3	1:E:70:LEU:HD13	1.99	0.44
1:E:12:GLY:H	1:E:35:ASN:HD22	1.64	0.44
1:B:164:LYS:HZ2	1:C:157:HIS:HE1	1.62	0.44
1:C:38:GLY:O	1:C:39:ASP:HB2	2.16	0.44
1:H:23:GLN:OE1	1:H:27:ARG:NH2	2.51	0.44
1:F:225:GLU:H	1:F:225:GLU:CD	2.21	0.44
1:C:75:GLU:HG3	1:C:76:ARG:HD2	2.00	0.44
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.83	0.44
1:F:61:LEU:HB2	1:F:110:LEU:HD23	2.00	0.43
1:B:73:LEU:CD2	1:B:77:GLU:HG2	2.49	0.43
1:F:186:LEU:HD22	1:F:221:PHE:CB	2.45	0.43
1:H:90:ILE:HG13	1:H:107:ILE:HD12	2.00	0.43
1:E:216:GLN:HE21	1:E:253:TRP:HE3	1.65	0.43
1:B:11:THR:O	1:B:87:ASN:HB3	2.18	0.43
1:A:162:LEU:O	1:A:166:VAL:HG23	2.18	0.43
1:H:104:TRP:CE3	1:H:151:ALA:HB2	2.54	0.43
1:A:90:ILE:CB	1:A:110:LEU:HD23	2.46	0.43
1:B:212:LEU:HD23	1:B:212:LEU:N	2.34	0.43
1:G:141:HIS:CE1	1:G:146:SER:OG	2.54	0.43
1:D:93:VAL:O	1:D:94:ALA:HB2	2.19	0.43
1:B:47:ILE:HG21	1:B:54:ALA:HB2	2.02	0.42
1:D:45:ALA:O	1:D:49:ARG:CD	2.66	0.42
1:H:23:GLN:HE22	1:H:225:GLU:HG3	1.84	0.42
1:D:60:ASP:H	1:D:66:GLN:NE2	2.18	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:223:THR:H	1:A:226:HIS:CD2	2.36	0.42
1:H:138:ALA:O	2:H:300:NAD:H6N	2.20	0.42
1:H:59:ALA:HA	1:H:66:GLN:HE21	1.84	0.42
1:F:86:ASN:HD22	1:F:136:ASN:HD21	1.68	0.42
1:B:196:ASP:O	1:B:197:ARG:HG2	2.19	0.42
1:F:8:ALA:HB3	1:F:32:ILE:HD13	2.00	0.42
1:D:89:GLY:HA2	1:D:110:LEU:HD13	2.02	0.42
1:F:12:GLY:H	1:F:35:ASN:ND2	2.18	0.42
1:F:25:LEU:HA	1:F:25:LEU:HD12	1.93	0.41
1:A:165:VAL:O	1:A:169:GLU:HG3	2.20	0.41
1:D:130:ASN:ND2	3:D:360:HOH:O	2.53	0.41
1:A:11:THR:O	1:A:87:ASN:HB3	2.19	0.41
1:B:59:ALA:CB	1:B:66:GLN:O	2.68	0.41
1:D:217:PRO:HD2	1:D:251:GLY:O	2.21	0.41
1:G:47:ILE:O	1:G:47:ILE:HD12	2.21	0.41
1:E:160:VAL:HG12	1:E:164:LYS:HE3	2.02	0.41
1:B:11:THR:HB	1:B:61:LEU:HD11	2.01	0.41
1:G:32:ILE:HG22	1:G:34:LEU:HG	2.02	0.41
1:A:10:VAL:HG12	1:A:13:SER:HB3	2.03	0.41
1:D:110:LEU:HB3	1:D:111:ASN:HD22	1.85	0.41
1:F:57:HIS:HB2	1:F:73:LEU:HD12	2.03	0.41
1:B:141:HIS:HD2	3:B:282:HOH:O	2.02	0.41
1:C:223:THR:H	1:C:226:HIS:CD2	2.39	0.41
1:C:90:ILE:H	1:C:111:ASN:HD21	1.68	0.41
1:H:110:LEU:O	1:H:114:ALA:HB3	2.21	0.41
1:B:8:ALA:HB3	1:B:32:ILE:HD13	2.02	0.41
1:A:215:LYS:HB3	1:A:253:TRP:CZ2	2.56	0.41
1:A:73:LEU:HD11	1:A:77:GLU:HG3	2.03	0.41
1:E:86:ASN:HB2	1:E:136:ASN:ND2	2.33	0.41
1:H:92:HIS:CE1	3:H:338:HOH:O	2.64	0.41
1:E:7:THR:HG21	1:E:78:PHE:HB2	2.03	0.41
1:F:123:LEU:N	1:F:124:PRO:CD	2.83	0.41
1:E:110:LEU:O	1:E:114:ALA:HB3	2.21	0.41
1:B:187:THR:HB	1:B:188:PRO:HD2	2.03	0.41
1:E:119:THR:HG23	1:E:134:ILE:HD13	2.01	0.41
1:C:186:LEU:HD22	1:C:221:PHE:CE1	2.55	0.41
1:D:90:ILE:HD11	1:D:106:LYS:HG3	2.03	0.40
1:A:182:PRO:HA	1:A:249:VAL:O	2.21	0.40
1:E:61:LEU:HD22	1:E:67:ILE:HG12	2.03	0.40
1:G:47:ILE:HD12	1:G:52:VAL:HG12	2.02	0.40
1:G:35:ASN:HA	1:G:57:HIS:O	2.21	0.40
1:F:111:ASN:HD22	1:F:111:ASN:N	2.19	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:57:HIS:HD2	1:C:59:ALA:N	2.17	0.40
1:E:149:LYS:HZ1	1:E:193:GLN:HE22	1.69	0.40
1:C:86:ASN:HD22	1:C:136:ASN:HD21	1.69	0.40
1:G:60:ASP:H	1:G:66:GLN:NE2	2.19	0.40
1:G:14:THR:CG2	1:G:37:PHE:O	2.60	0.40
1:F:182:PRO:HB2	2:F:300:NAD:C5N	2.51	0.40
1:C:121:LEU:HD23	1:C:121:LEU:HA	1.93	0.40
1:B:203:ASP:HA	1:B:204:PRO:HD2	1.92	0.40
1:D:57:HIS:HE1	3:D:363:HOH:O	2.05	0.40

All (1) 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	Distance(Å)	Clash(Å)
3:E:336:HOH:O	3:G:332:HOH:O[2_555]	1.98	0.22

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	246/255 (96%)	237 (96%)	9 (4%)	0	100	100
1	B	248/255 (97%)	230 (93%)	15 (6%)	3 (1%)	19	9
1	C	239/255 (94%)	224 (94%)	13 (5%)	2 (1%)	27	17
1	D	253/255 (99%)	244 (96%)	8 (3%)	1 (0%)	43	35
1	E	245/255 (96%)	233 (95%)	11 (4%)	1 (0%)	43	35
1	F	234/255 (92%)	226 (97%)	8 (3%)	0	100	100
1	G	247/255 (97%)	237 (96%)	7 (3%)	3 (1%)	19	9
1	H	236/255 (92%)	220 (93%)	14 (6%)	2 (1%)	27	17
All	All	1948/2040 (96%)	1851 (95%)	85 (4%)	12 (1%)	33	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	39	ASP
1	H	46	GLU
1	H	47	ILE
1	G	207	ALA
1	B	196	ASP
1	B	130	ASN
1	B	197	ARG
1	G	138	ALA
1	C	131	TRP
1	D	202	GLY
1	E	206	GLN
1	G	206	GLN

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	188/189 (100%)	175 (93%)	13 (7%)	22	14
1	B	188/189 (100%)	175 (93%)	13 (7%)	22	14
1	C	181/189 (96%)	159 (88%)	22 (12%)	7	3
1	D	189/189 (100%)	174 (92%)	15 (8%)	18	10
1	E	186/189 (98%)	166 (89%)	20 (11%)	9	4
1	F	176/189 (93%)	161 (92%)	15 (8%)	15	9
1	G	187/189 (99%)	169 (90%)	18 (10%)	12	6
1	H	178/189 (94%)	168 (94%)	10 (6%)	30	22
All	All	1473/1512 (97%)	1347 (91%)	126 (9%)	15	8

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	23	GLN
1	A	25	LEU
1	A	27	ARG
1	A	53	LYS
1	A	98	GLN

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Mol	Chain	Res	Type
1	A	106	LYS
1	A	111	ASN
1	A	192	LYS
1	A	205	LEU
1	A	212	LEU
1	A	217	PRO
1	A	230	LEU
1	B	25	LEU
1	B	52	VAL
1	B	53	LYS
1	B	73	LEU
1	B	76	ARG
1	B	106	LYS
1	B	186	LEU
1	B	192	LYS
1	B	194	ILE
1	B	195	ASP
1	B	197	ARG
1	B	205	LEU
1	B	225	GLU
1	C	15	SER
1	C	23	GLN
1	C	25	LEU
1	C	34	LEU
1	C	47	ILE
1	C	49	ARG
1	C	52	VAL
1	C	76	ARG
1	C	102	GLU
1	C	110	LEU
1	C	111	ASN
1	C	189	LEU
1	C	190	VAL
1	C	191	GLN
1	C	192	LYS
1	C	193	GLN
1	C	210	ASP
1	C	211	LEU
1	C	212	LEU
1	C	214	GLU
1	C	230	LEU
1	C	232	LEU

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Mol	Chain	Res	Type
1	D	2	THR
1	D	14	THR
1	D	15	SER
1	D	23	GLN
1	D	25	LEU
1	D	34	LEU
1	D	76	ARG
1	D	101	LEU
1	D	102	GLU
1	D	110	LEU
1	D	111	ASN
1	D	188	PRO
1	D	205	LEU
1	D	230	LEU
1	D	232	LEU
1	E	6	LYS
1	E	14	THR
1	E	25	LEU
1	E	27	ARG
1	E	42	PRO
1	E	47	ILE
1	E	49	ARG
1	E	75	GLU
1	E	98	GLN
1	E	103	SER
1	E	110	LEU
1	E	120	ARG
1	E	124	PRO
1	E	130	ASN
1	E	192	LYS
1	E	206	GLN
1	E	212	LEU
1	E	225	GLU
1	E	230	LEU
1	E	232	LEU
1	F	2	THR
1	F	23	GLN
1	F	25	LEU
1	F	49	ARG
1	F	52	VAL
1	F	73	LEU
1	F	76	ARG

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Mol	Chain	Res	Type
1	F	97	GLU
1	F	101	LEU
1	F	110	LEU
1	F	111	ASN
1	F	140	VAL
1	F	186	LEU
1	F	212	LEU
1	F	230	LEU
1	G	2	THR
1	G	13	SER
1	G	14	THR
1	G	25	LEU
1	G	47	ILE
1	G	52	VAL
1	G	96	VAL
1	G	106	LYS
1	G	110	LEU
1	G	111	ASN
1	G	192	LYS
1	G	208	GLN
1	G	210	ASP
1	G	211	LEU
1	G	212	LEU
1	G	214	GLU
1	G	230	LEU
1	G	232	LEU
1	H	23	GLN
1	H	25	LEU
1	H	46	GLU
1	H	101	LEU
1	H	102	GLU
1	H	110	LEU
1	H	111	ASN
1	H	206	GLN
1	H	212	LEU
1	H	230	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	35	ASN

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Mol	Chain	Res	Type
1	A	66	GLN
1	A	111	ASN
1	A	136	ASN
1	A	141	HIS
1	A	216	GLN
1	A	226	HIS
1	A	256	GLN
1	B	35	ASN
1	B	66	GLN
1	B	111	ASN
1	B	136	ASN
1	B	141	HIS
1	B	216	GLN
1	B	226	HIS
1	B	256	GLN
1	C	35	ASN
1	C	57	HIS
1	C	66	GLN
1	C	111	ASN
1	C	136	ASN
1	C	141	HIS
1	C	157	HIS
1	C	193	GLN
1	C	216	GLN
1	D	35	ASN
1	D	57	HIS
1	D	66	GLN
1	D	92	HIS
1	D	98	GLN
1	D	111	ASN
1	D	130	ASN
1	D	136	ASN
1	D	141	HIS
1	D	157	HIS
1	D	193	GLN
1	D	216	GLN
1	E	35	ASN
1	E	57	HIS
1	E	66	GLN
1	E	98	GLN
1	E	111	ASN
1	E	136	ASN

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Mol	Chain	Res	Type
1	E	141	HIS
1	E	157	HIS
1	E	193	GLN
1	E	216	GLN
1	E	226	HIS
1	E	256	GLN
1	F	35	ASN
1	F	66	GLN
1	F	111	ASN
1	F	136	ASN
1	F	141	HIS
1	F	216	GLN
1	G	35	ASN
1	G	57	HIS
1	G	66	GLN
1	G	111	ASN
1	G	136	ASN
1	G	141	HIS
1	G	157	HIS
1	G	193	GLN
1	G	216	GLN
1	H	35	ASN
1	H	66	GLN
1	H	92	HIS
1	H	111	ASN
1	H	130	ASN
1	H	136	ASN
1	H	141	HIS
1	H	216	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	C	300	-	48,48,48	1.65	6 (12%)	73,73,73	2.04	10 (13%)
2	NAD	D	300	-	48,48,48	1.34	8 (16%)	73,73,73	2.42	19 (26%)
2	NAD	E	300	-	48,48,48	1.48	8 (16%)	73,73,73	2.07	11 (15%)
2	NAD	F	300	-	48,48,48	1.59	8 (16%)	73,73,73	2.28	15 (20%)
2	NAD	G	300	-	48,48,48	1.46	5 (10%)	73,73,73	1.90	14 (19%)
2	NAD	H	300	-	48,48,48	1.61	7 (14%)	73,73,73	2.30	13 (17%)

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	C	300	-	-	0/30/62/62	0/3/5/5
2	NAD	D	300	-	-	0/30/62/62	0/3/5/5
2	NAD	E	300	-	-	0/30/62/62	0/3/5/5
2	NAD	F	300	-	-	0/30/62/62	0/3/5/5
2	NAD	G	300	-	-	0/30/62/62	0/3/5/5
2	NAD	H	300	-	-	0/30/62/62	0/3/5/5

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	NAD	O7N-C7N	8.03	1.43	1.24
2	H	300	NAD	O7N-C7N	6.49	1.39	1.24
2	F	300	NAD	O7N-C7N	5.79	1.37	1.24
2	G	300	NAD	O7N-C7N	5.25	1.36	1.24
2	E	300	NAD	O7N-C7N	5.14	1.36	1.24
2	G	300	NAD	C2A-N1A	4.16	1.42	1.33
2	H	300	NAD	C2N-N1N	3.83	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	300	NAD	C2A-N1A	3.71	1.41	1.33
2	F	300	NAD	C2N-N1N	3.39	1.39	1.35
2	F	300	NAD	C2A-N3A	3.35	1.38	1.32
2	F	300	NAD	C2A-N1A	3.31	1.40	1.33
2	D	300	NAD	O7N-C7N	3.29	1.31	1.24
2	D	300	NAD	C2N-C3N	-3.28	1.34	1.38
2	C	300	NAD	C2A-N3A	3.28	1.38	1.32
2	E	300	NAD	C2N-N1N	3.15	1.39	1.35
2	H	300	NAD	C2A-N3A	3.04	1.38	1.32
2	H	300	NAD	C2N-C3N	3.02	1.43	1.38
2	F	300	NAD	PA-O3	2.87	1.65	1.59
2	G	300	NAD	O4B-C1B	2.86	1.45	1.41
2	H	300	NAD	C2A-N1A	2.84	1.39	1.33
2	C	300	NAD	C2A-N1A	2.78	1.39	1.33
2	E	300	NAD	C5N-C4N	2.75	1.45	1.39
2	E	300	NAD	PA-O3	2.68	1.64	1.59
2	C	300	NAD	PA-O3	2.67	1.64	1.59
2	G	300	NAD	PA-O3	2.63	1.64	1.59
2	F	300	NAD	C2N-C3N	2.54	1.42	1.38
2	F	300	NAD	O4D-C1D	2.40	1.45	1.41
2	H	300	NAD	C8A-N9A	2.39	1.40	1.36
2	E	300	NAD	C2A-N3A	2.36	1.36	1.32
2	D	300	NAD	C8A-N9A	2.31	1.40	1.36
2	C	300	NAD	C2N-N1N	2.29	1.38	1.35
2	D	300	NAD	O4D-C1D	2.27	1.44	1.41
2	E	300	NAD	PN-O3	-2.27	1.55	1.60
2	E	300	NAD	C3N-C7N	2.19	1.54	1.50
2	D	300	NAD	O4B-C1B	2.15	1.44	1.41
2	D	300	NAD	C2A-N3A	2.15	1.36	1.32
2	H	300	NAD	C4A-N3A	2.15	1.38	1.35
2	F	300	NAD	C8A-N9A	2.15	1.39	1.36
2	E	300	NAD	O4D-C1D	2.10	1.44	1.41
2	G	300	NAD	C2A-N3A	2.08	1.36	1.32
2	C	300	NAD	O4B-C1B	2.08	1.44	1.41
2	D	300	NAD	PA-O2A	-2.02	1.46	1.55

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	NAD	N3A-C2A-N1A	-13.28	117.61	128.71
2	D	300	NAD	C3N-C7N-N7N	11.40	130.74	117.77
2	F	300	NAD	O4D-C1D-N1N	10.35	118.54	107.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	NAD	N3A-C2A-N1A	-10.26	120.13	128.71
2	E	300	NAD	N3A-C2A-N1A	-9.31	120.93	128.71
2	F	300	NAD	N3A-C2A-N1A	-8.92	121.25	128.71
2	E	300	NAD	C3N-C7N-N7N	8.49	127.43	117.77
2	C	300	NAD	O4D-C1D-N1N	8.19	116.33	107.95
2	D	300	NAD	N3A-C2A-N1A	-7.65	122.31	128.71
2	G	300	NAD	O4B-C1B-N9A	6.10	114.11	108.44
2	D	300	NAD	O7N-C7N-N7N	-5.97	113.97	122.59
2	H	300	NAD	O3-PN-O1N	-5.87	94.81	108.83
2	F	300	NAD	C3N-C7N-N7N	5.63	124.18	117.77
2	G	300	NAD	N3A-C2A-N1A	-5.60	124.03	128.71
2	E	300	NAD	O7N-C7N-C3N	-5.24	113.67	119.58
2	E	300	NAD	O4D-C1D-N1N	5.15	113.22	107.95
2	G	300	NAD	O3-PN-O1N	-5.10	96.64	108.83
2	G	300	NAD	O7N-C7N-C3N	-5.09	113.83	119.58
2	H	300	NAD	C1B-N9A-C4A	-4.65	118.60	126.64
2	D	300	NAD	C3B-C2B-C1B	-4.60	93.70	100.91
2	H	300	NAD	C3N-C7N-N7N	4.55	122.94	117.77
2	G	300	NAD	N3A-C4A-N9A	4.53	133.62	125.43
2	G	300	NAD	C3N-C7N-N7N	4.45	122.84	117.77
2	C	300	NAD	N3A-C4A-N9A	4.39	133.37	125.43
2	F	300	NAD	N3A-C4A-N9A	4.11	132.85	125.43
2	D	300	NAD	N3A-C4A-N9A	4.06	132.75	125.43
2	D	300	NAD	O7N-C7N-C3N	-3.90	115.19	119.58
2	F	300	NAD	O4B-C1B-N9A	3.78	111.95	108.44
2	D	300	NAD	C4D-O4D-C1D	-3.75	105.67	109.75
2	H	300	NAD	C8A-N9A-C4A	3.74	109.75	106.90
2	D	300	NAD	O3D-C3D-C2D	-3.45	100.62	111.83
2	F	300	NAD	C8A-N9A-C4A	3.40	109.50	106.90
2	D	300	NAD	C8A-N9A-C4A	3.33	109.44	106.90
2	H	300	NAD	C2A-N1A-C6A	3.28	124.70	118.77
2	F	300	NAD	PN-O5D-C5D	3.28	131.58	120.24
2	E	300	NAD	N3A-C4A-N9A	3.22	131.25	125.43
2	F	300	NAD	O7N-C7N-N7N	-3.03	118.21	122.59
2	G	300	NAD	C6A-C5A-C4A	3.03	122.81	117.25
2	C	300	NAD	O4B-C1B-N9A	2.98	111.21	108.44
2	G	300	NAD	C2D-C1D-N1N	2.97	118.89	113.86
2	F	300	NAD	C6N-N1N-C2N	-2.92	118.74	122.04
2	G	300	NAD	C8A-N9A-C4A	2.91	109.12	106.90
2	D	300	NAD	N7A-C8A-N9A	-2.81	106.41	114.36
2	D	300	NAD	O4D-C1D-C2D	-2.81	102.46	106.77
2	D	300	NAD	O3B-C3B-C4B	-2.74	103.00	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	300	NAD	N7A-C8A-N9A	-2.73	106.63	114.36
2	E	300	NAD	O7N-C7N-N7N	-2.72	118.66	122.59
2	F	300	NAD	C1B-N9A-C4A	-2.69	121.98	126.64
2	H	300	NAD	C8A-N9A-C1B	2.67	131.64	126.38
2	C	300	NAD	C8A-N9A-C4A	2.66	108.93	106.90
2	G	300	NAD	N7A-C8A-N9A	-2.65	106.86	114.36
2	F	300	NAD	O3-PN-O1N	-2.65	102.50	108.83
2	C	300	NAD	C2D-C1D-N1N	-2.62	109.42	113.86
2	G	300	NAD	PN-O5D-C5D	2.61	129.28	120.24
2	G	300	NAD	O5B-PA-O1A	-2.51	99.55	109.37
2	H	300	NAD	C4D-O4D-C1D	2.51	112.47	109.75
2	G	300	NAD	C5A-C4A-N3A	-2.50	120.25	125.70
2	D	300	NAD	O3-PN-O1N	-2.47	102.93	108.83
2	H	300	NAD	N3A-C4A-N9A	2.43	129.82	125.43
2	D	300	NAD	C5A-C6A-N6A	2.38	126.11	120.72
2	E	300	NAD	O3B-C3B-C2B	-2.35	104.18	111.83
2	D	300	NAD	N6A-C6A-N1A	-2.34	114.77	119.36
2	H	300	NAD	O2A-PA-O3	2.33	116.21	105.14
2	E	300	NAD	C2A-N1A-C6A	2.33	122.98	118.77
2	E	300	NAD	O3-PN-O5D	-2.32	92.06	101.36
2	D	300	NAD	C4A-C5A-N7A	-2.31	107.54	109.52
2	G	300	NAD	C3B-C2B-C1B	-2.30	97.31	100.91
2	F	300	NAD	N7A-C8A-N9A	-2.29	107.89	114.36
2	H	300	NAD	O4B-C1B-N9A	2.25	110.53	108.44
2	E	300	NAD	C4D-O4D-C1D	-2.24	107.32	109.75
2	D	300	NAD	C8A-N7A-C5A	2.21	110.44	103.58
2	H	300	NAD	O7N-C7N-N7N	-2.17	119.45	122.59
2	F	300	NAD	O2B-C2B-C3B	2.17	118.90	111.83
2	E	300	NAD	O2B-C2B-C3B	2.11	118.69	111.83
2	C	300	NAD	PN-O3-PA	-2.10	123.94	132.95
2	D	300	NAD	C5N-C6N-N1N	-2.07	116.94	120.43
2	C	300	NAD	O5D-PN-O1N	2.07	117.39	108.61
2	F	300	NAD	O5D-PN-O1N	-2.06	99.85	108.61
2	D	300	NAD	C5A-C4A-N3A	-2.06	121.22	125.70
2	C	300	NAD	C5A-C4A-N3A	-2.03	121.27	125.70
2	C	300	NAD	N7A-C8A-N9A	-2.03	108.63	114.36
2	F	300	NAD	O4D-C1D-C2D	-2.01	103.70	106.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	250/255 (98%)	0.79	35 (14%) 3 3	36, 42, 52, 60	0
1	B	252/255 (98%)	0.69	22 (8%) 10 10	35, 42, 48, 59	0
1	C	243/255 (95%)	1.17	49 (20%) 2 2	35, 42, 50, 57	0
1	D	255/255 (100%)	0.74	37 (14%) 3 3	37, 42, 50, 59	0
1	E	249/255 (97%)	0.84	37 (14%) 3 3	36, 42, 48, 57	0
1	F	238/255 (93%)	0.85	34 (14%) 3 3	35, 42, 50, 55	0
1	G	251/255 (98%)	0.95	41 (16%) 2 2	35, 42, 49, 56	0
1	H	240/255 (94%)	0.85	40 (16%) 2 2	36, 42, 53, 63	0
All	All	1978/2040 (96%)	0.86	295 (14%) 3 3	35, 42, 50, 63	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	ALA	10.2
1	E	205	LEU	9.2
1	C	190	VAL	8.8
1	G	199	ALA	7.7
1	C	189	LEU	7.6
1	E	198	ALA	7.4
1	C	2	THR	6.9
1	C	194	ILE	6.8
1	D	201	GLY	6.5
1	G	204	PRO	6.4
1	D	200	ASN	6.2
1	H	205	LEU	6.1
1	C	38	GLY	6.1
1	G	205	LEU	6.1
1	H	188	PRO	6.1
1	E	207	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	194	ILE	6.0
1	A	194	ILE	5.9
1	B	198	ALA	5.7
1	F	159	VAL	5.3
1	B	203	ASP	5.3
1	G	194	ILE	5.1
1	B	202	GLY	5.1
1	F	189	LEU	5.1
1	B	194	ILE	5.0
1	D	199	ALA	4.9
1	G	206	GLN	4.9
1	C	193	GLN	4.7
1	C	41	ALA	4.7
1	H	204	PRO	4.6
1	C	15	SER	4.5
1	A	195	ASP	4.4
1	B	197	ARG	4.4
1	F	211	LEU	4.4
1	B	204	PRO	4.3
1	A	52	VAL	4.2
1	H	206	GLN	4.2
1	H	4	LYS	4.2
1	H	76	ARG	4.2
1	A	196	ASP	4.2
1	D	137	ILE	4.1
1	H	159	VAL	4.1
1	D	198	ALA	4.1
1	F	186	LEU	4.1
1	A	54	ALA	4.1
1	C	55	VAL	4.1
1	E	159	VAL	4.1
1	B	207	ALA	4.1
1	E	76	ARG	4.1
1	E	196	ASP	4.0
1	C	76	ARG	4.0
1	D	160	VAL	4.0
1	G	2	THR	4.0
1	D	159	VAL	4.0
1	G	207	ALA	3.9
1	G	159	VAL	3.9
1	G	160	VAL	3.9
1	C	211	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	48	ALA	3.9
1	C	188	PRO	3.9
1	F	2	THR	3.9
1	E	155	ALA	3.8
1	A	197	ARG	3.8
1	C	3	LEU	3.8
1	A	206	GLN	3.7
1	F	208	GLN	3.7
1	C	186	LEU	3.7
1	B	205	LEU	3.7
1	C	209	HIS	3.7
1	G	135	ILE	3.7
1	H	52	VAL	3.7
1	A	204	PRO	3.6
1	D	162	LEU	3.6
1	G	76	ARG	3.6
1	E	160	VAL	3.6
1	H	2	THR	3.6
1	F	188	PRO	3.6
1	C	208	GLN	3.6
1	B	190	VAL	3.5
1	E	154	ALA	3.5
1	H	48	ALA	3.5
1	D	135	ILE	3.5
1	D	180	ILE	3.5
1	B	189	LEU	3.4
1	A	49	ARG	3.4
1	D	138	ALA	3.4
1	E	197	ARG	3.4
1	C	81	VAL	3.4
1	H	155	ALA	3.4
1	A	205	LEU	3.3
1	D	112	LEU	3.3
1	F	160	VAL	3.3
1	H	160	VAL	3.3
1	A	65	ALA	3.3
1	D	179	ALA	3.3
1	H	186	LEU	3.3
1	F	115	VAL	3.2
1	D	163	THR	3.2
1	D	85	VAL	3.2
1	D	181	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	163	THR	3.2
1	G	55	VAL	3.2
1	H	80	GLY	3.2
1	B	160	VAL	3.2
1	A	203	ASP	3.1
1	C	128	ALA	3.1
1	F	162	LEU	3.1
1	A	46	GLU	3.1
1	F	209	HIS	3.1
1	G	163	THR	3.1
1	G	137	ILE	3.1
1	B	159	VAL	3.1
1	C	47	ILE	3.1
1	H	208	GLN	3.0
1	C	42	PRO	3.0
1	D	155	ALA	3.0
1	F	158	GLY	3.0
1	G	197	ARG	3.0
1	C	39	ASP	3.0
1	F	38	GLY	3.0
1	E	206	GLN	3.0
1	G	196	ASP	3.0
1	C	192	LYS	3.0
1	D	136	ASN	3.0
1	C	54	ALA	3.0
1	F	112	LEU	3.0
1	H	158	GLY	3.0
1	F	137	ILE	3.0
1	H	207	ALA	3.0
1	E	162	LEU	3.0
1	C	160	VAL	2.9
1	D	115	VAL	2.9
1	E	138	ALA	2.9
1	F	155	ALA	2.9
1	D	84	LEU	2.9
1	A	192	LYS	2.9
1	G	155	ALA	2.9
1	G	53	LYS	2.9
1	E	137	ILE	2.9
1	C	64	VAL	2.9
1	H	144	VAL	2.9
1	E	209	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	208	GLN	2.8
1	E	143	LEU	2.8
1	C	72	ALA	2.8
1	F	85	VAL	2.8
1	D	142	GLY	2.8
1	G	162	LEU	2.8
1	E	158	GLY	2.8
1	A	189	LEU	2.8
1	A	211	LEU	2.8
1	D	246	ALA	2.8
1	B	192	LYS	2.8
1	G	192	LYS	2.8
1	C	73	LEU	2.7
1	H	112	LEU	2.7
1	D	202	GLY	2.7
1	B	196	ASP	2.7
1	D	144	VAL	2.7
1	G	143	LEU	2.7
1	A	51	GLY	2.7
1	D	87	ASN	2.7
1	C	52	VAL	2.7
1	A	158	GLY	2.7
1	H	142	GLY	2.7
1	C	80	GLY	2.7
1	E	153	VAL	2.7
1	G	177	CYS	2.7
1	C	137	ILE	2.6
1	G	179	ALA	2.6
1	H	161	GLY	2.6
1	G	85	VAL	2.6
1	B	74	ALA	2.6
1	F	135	ILE	2.6
1	F	210	ASP	2.6
1	G	134	ILE	2.6
1	A	186	LEU	2.6
1	A	187	THR	2.6
1	D	86	ASN	2.6
1	E	5	GLY	2.6
1	H	39	ASP	2.6
1	A	207	ALA	2.6
1	H	45	ALA	2.6
1	A	42	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	85	VAL	2.5
1	E	190	VAL	2.5
1	B	195	ASP	2.5
1	G	195	ASP	2.5
1	B	143	LEU	2.5
1	H	154	ALA	2.5
1	A	190	VAL	2.5
1	E	144	VAL	2.5
1	C	158	GLY	2.5
1	G	208	GLN	2.5
1	C	4	LYS	2.5
1	C	69	ALA	2.5
1	F	161	GLY	2.5
1	H	51	GLY	2.5
1	F	49	ARG	2.5
1	A	208	GLN	2.5
1	C	207	ALA	2.5
1	A	2	THR	2.4
1	F	136	ASN	2.4
1	D	140	VAL	2.4
1	G	166	VAL	2.4
1	G	180	ILE	2.4
1	C	37	PHE	2.4
1	C	49	ARG	2.4
1	E	246	ALA	2.4
1	C	28	ALA	2.4
1	C	74	ALA	2.4
1	G	65	ALA	2.4
1	E	192	LYS	2.4
1	D	247	TRP	2.4
1	E	179	ALA	2.4
1	C	92	HIS	2.4
1	A	53	LYS	2.4
1	G	77	GLU	2.4
1	G	190	VAL	2.3
1	E	163	THR	2.3
1	G	52	VAL	2.3
1	A	50	HIS	2.3
1	A	45	ALA	2.3
1	E	135	ILE	2.3
1	H	163	THR	2.3
1	F	179	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	180	ILE	2.3
1	A	160	VAL	2.3
1	D	153	VAL	2.3
1	H	115	VAL	2.3
1	H	41	ALA	2.3
1	H	138	ALA	2.3
1	A	47	ILE	2.3
1	C	67	ILE	2.3
1	G	39	ASP	2.3
1	B	155	ALA	2.3
1	F	154	ALA	2.3
1	E	157	HIS	2.3
1	F	245	ALA	2.2
1	G	246	ALA	2.2
1	E	80	GLY	2.2
1	D	204	PRO	2.2
1	E	181	CYS	2.2
1	C	138	ALA	2.2
1	E	85	VAL	2.2
1	E	195	ASP	2.2
1	H	114	ALA	2.2
1	F	96	VAL	2.2
1	A	37	PHE	2.2
1	H	209	HIS	2.2
1	D	130	ASN	2.2
1	B	73	LEU	2.2
1	C	43	ALA	2.2
1	H	86	ASN	2.2
1	C	63	ASP	2.2
1	E	210	ASP	2.2
1	D	158	GLY	2.2
1	G	186	LEU	2.2
1	B	90	ILE	2.2
1	G	210	ASP	2.2
1	C	191	GLN	2.1
1	G	193	GLN	2.1
1	A	85	VAL	2.1
1	H	55	VAL	2.1
1	H	143	LEU	2.1
1	H	179	ALA	2.1
1	H	157	HIS	2.1
1	H	11	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	159	VAL	2.1
1	A	76	ARG	2.1
1	D	143	LEU	2.1
1	F	177	CYS	2.1
1	D	157	HIS	2.1
1	C	163	THR	2.1
1	F	77	GLU	2.1
1	A	161	GLY	2.1
1	G	161	GLY	2.1
1	C	87	ASN	2.1
1	H	151	ALA	2.1
1	D	156	LYS	2.1
1	D	205	LEU	2.0
1	H	162	LEU	2.0
1	F	11	THR	2.0
1	H	187	THR	2.0
1	E	136	ASN	2.0
1	A	209	HIS	2.0
1	F	214	GLU	2.0
1	E	72	ALA	2.0
1	E	84	LEU	2.0
1	F	86	ASN	2.0
1	F	207	ALA	2.0
1	D	242	VAL	2.0
1	G	115	VAL	2.0
1	C	8	ALA	2.0
1	B	158	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAD	C	300	44/44	0.17	-0.39	47,62,73,77	0
2	NAD	F	300	44/44	0.15	-0.47	39,51,56,59	0
2	NAD	D	300	44/44	0.11	-0.84	25,35,41,44	0
2	NAD	H	300	44/44	0.09	-1.06	33,42,47,51	0
2	NAD	E	300	44/44	0.08	-1.12	30,39,45,49	0
2	NAD	G	300	44/44	0.09	-1.13	35,42,48,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.