



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 08:08 PM GMT

PDB ID : 1T2F
Title : Human B lactate dehydrogenase complexed with NAD⁺ and 4-hydroxy-1,2,5-oxadiazole-3-carboxylic acid
Authors : Cameron, A.; Read, J.; Tranter, R.; Winter, V.J.; Sessions, R.B.; Brady, R.L.; Vivas, L.; Easton, A.; Kendrick, H.; Croft, S.L.; Barros, D.; Lavandera, J.L.; Martin, J.J.; Risco, F.; Garcia-Ochoa, S.; Gamo, F.J.; Sanz, L.; Leon, L.; Ruiz, J.R.; Gabarro, R.; Mallo, A.; De Las Heras, F.G.
Deposited on : 2004-04-21
Resolution : 3.00 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>

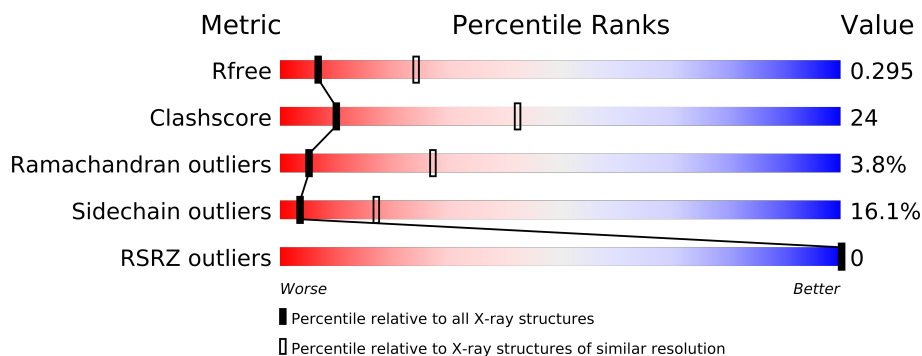
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	333	
1	B	333	
1	C	333	
1	D	333	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10665 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.

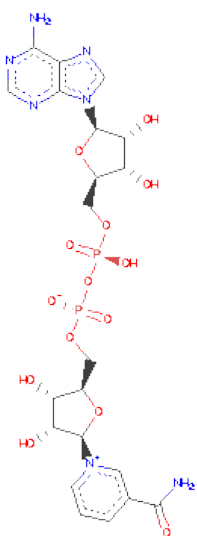
- Molecule 1 is a protein called L-lactate dehydrogenase B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	51	0	0
			2555	1627	430	484	14			
1	B	332	Total	C	N	O	S	71	0	0
			2555	1627	430	484	14			
1	C	332	Total	C	N	O	S	65	0	0
			2555	1627	430	484	14			
1	D	332	Total	C	N	O	S	78	0	0
			2555	1627	430	484	14			

There are 4 discrepancies between the modelled and reference sequences:

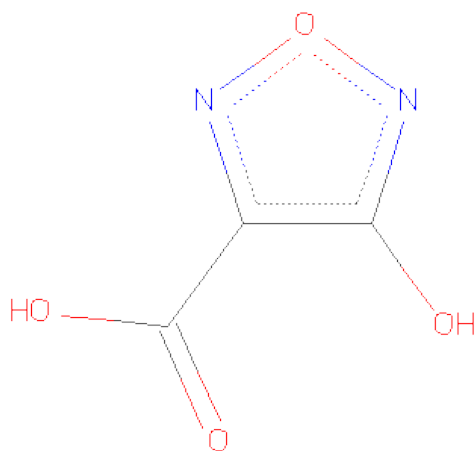
Chain	Residue	Modelled	Actual	Comment	Reference
A	332	PHE	ASP	ENGINEERED	UNP P07195
B	332	PHE	ASP	ENGINEERED	UNP P07195
C	332	PHE	ASP	ENGINEERED	UNP P07195
D	332	PHE	ASP	ENGINEERED	UNP P07195

- 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		

- Molecule 3 is 4-HYDROXY-1,2,5-OXADIAZOLE-3-CARBOXYLICACID (three-letter code: OXQ) (formula: C₃H₂N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	3	2	4		
3	B	1	Total	C	N	O	0	0
			9	3	2	4		
3	C	1	Total	C	N	O	0	0
			9	3	2	4		
3	D	1	Total	C	N	O	0	0
			9	3	2	4		

- Molecule 4 is water.

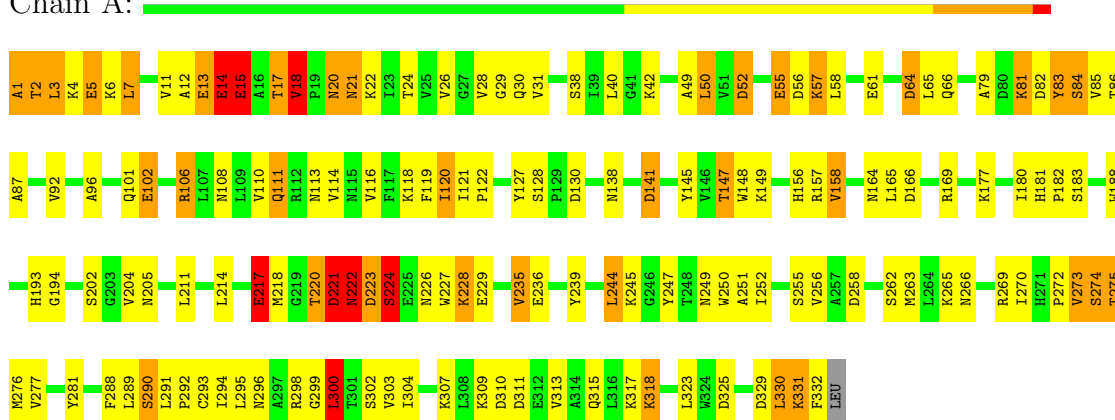
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		
4	B	76	Total	O	0	0
			76	76		
4	C	48	Total	O	0	0
			48	48		
4	D	43	Total	O	0	0
			43	43		

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.

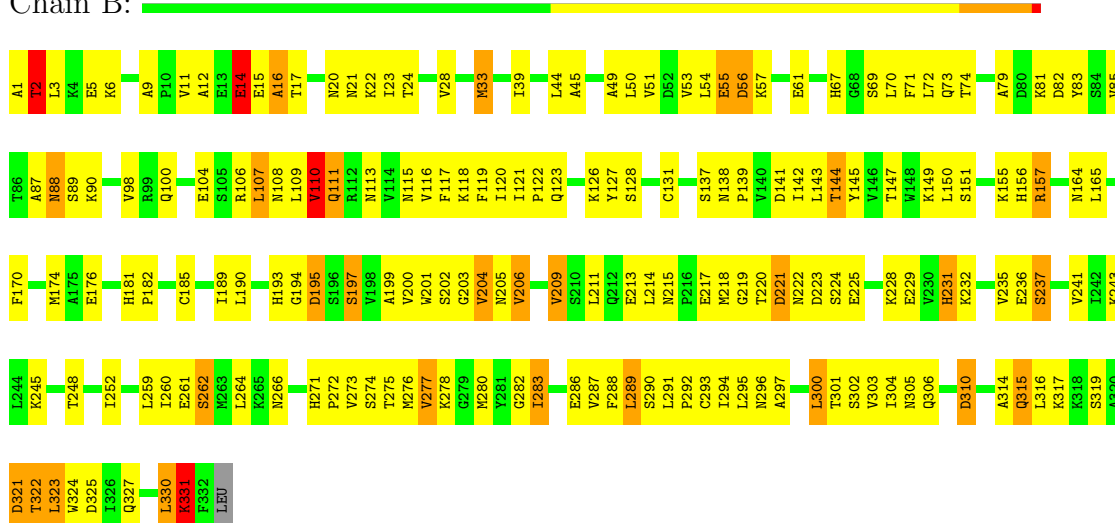
• Molecule 1: L-lactate dehydrogenase B chain

Chain A:



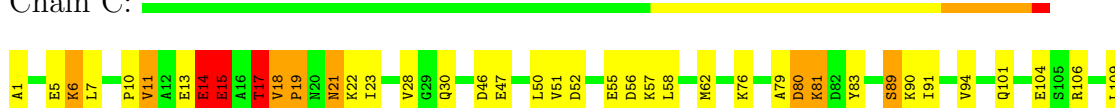
• Molecule 1: L-lactate dehydrogenase B chain

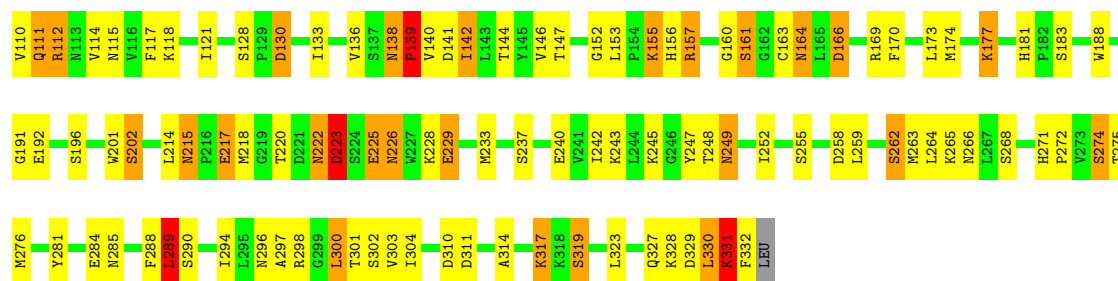
Chain B:



• Molecule 1: L-lactate dehydrogenase B chain

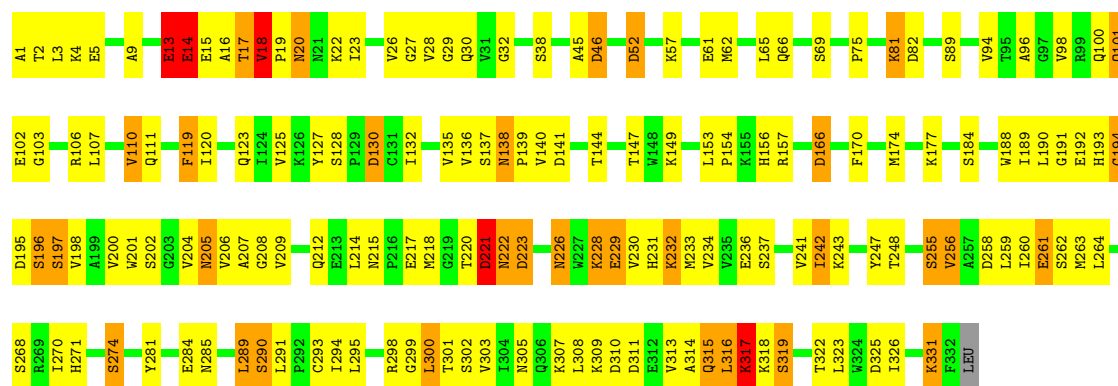
Chain C:





• Molecule 1: L-lactate dehydrogenase B chain

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.40Å 160.44Å 59.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 3.00 28.90 – 2.99	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.88-3.00) 90.3 (28.90-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.321 0.201 , 0.295	Depositor DCC
R_{free} test set	1242 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 24666 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10665	wwPDB-VP
Average B, all atoms (Å ²)	56.0	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 46.79 % 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 1.0889e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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: OXQ, 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	1.26	8/2597 (0.3%)	1.28	18/3520 (0.5%)
1	B	1.19	6/2597 (0.2%)	1.19	24/3520 (0.7%)
1	C	1.24	8/2597 (0.3%)	1.28	29/3520 (0.8%)
1	D	1.49	13/2597 (0.5%)	1.52	36/3520 (1.0%)
All	All	1.30	35/10388 (0.3%)	1.32	107/14080 (0.8%)

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	A	1	2
1	B	1	3
1	C	2	2
1	D	4	0
All	All	8	7

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	GLU	CA-CB	-33.15	0.81	1.53
1	D	119	PHE	CB-CG	29.10	2.00	1.51
1	A	222	ASN	CA-CB	27.49	2.24	1.53
1	D	318	LYS	CA-CB	-27.04	0.94	1.53
1	D	217	GLU	CB-CG	-26.53	1.01	1.52
1	B	217	GLU	CA-CB	-26.11	0.96	1.53
1	A	221	ASP	CA-CB	-23.00	1.03	1.53
1	B	221	ASP	CA-CB	-19.59	1.10	1.53
1	D	229	GLU	CB-CG	-18.69	1.16	1.52
1	C	317	LYS	CG-CD	16.33	2.08	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	331	LYS	CA-CB	-16.11	1.18	1.53
1	C	229	GLU	CB-CG	16.04	1.82	1.52
1	B	145	TYR	CB-CG	15.21	1.74	1.51
1	D	214	LEU	CA-CB	-15.10	1.19	1.53
1	D	13	GLU	CB-CG	14.89	1.80	1.52
1	D	4	LYS	CG-CD	-12.71	1.09	1.52
1	A	14	GLU	CA-CB	12.37	1.81	1.53
1	D	284	GLU	CA-CB	-12.26	1.26	1.53
1	A	228	LYS	CB-CG	-12.07	1.20	1.52
1	B	14	GLU	CA-CB	-12.00	1.27	1.53
1	B	225	GLU	CA-CB	-11.14	1.29	1.53
1	C	217	GLU	CA-CB	-9.23	1.33	1.53
1	C	331	LYS	CA-CB	9.10	1.74	1.53
1	A	217	GLU	CA-CB	-7.97	1.36	1.53
1	D	221	ASP	CA-CB	7.70	1.70	1.53
1	A	118	LYS	CB-CG	7.58	1.73	1.52
1	A	331	LYS	CA-CB	-7.02	1.38	1.53
1	D	81	LYS	CG-CD	7.01	1.76	1.52
1	D	307	LYS	CB-CG	6.82	1.71	1.52
1	D	228	LYS	CB-CG	-6.72	1.34	1.52
1	C	298	ARG	CA-CB	6.22	1.67	1.53
1	D	317	LYS	CA-CB	-5.71	1.41	1.53
1	C	101	GLN	CA-CB	-5.08	1.42	1.53
1	C	228	LYS	CA-CB	-5.05	1.42	1.53
1	A	298	ARG	CB-CG	-5.04	1.39	1.52

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ASP	CA-CB-CG	27.37	173.62	113.40
1	D	318	LYS	CA-CB-CG	27.25	173.35	113.40
1	D	119	PHE	CB-CG-CD2	20.86	135.40	120.80
1	A	221	ASP	N-CA-CB	20.71	147.88	110.60
1	D	331	LYS	N-CA-CB	20.29	147.12	110.60
1	C	6	LYS	CA-CB-CG	19.84	157.04	113.40
1	D	119	PHE	CB-CG-CD1	-19.63	107.06	120.80
1	D	221	ASP	CB-CA-C	19.38	149.16	110.40
1	D	317	LYS	CA-CB-CG	18.01	153.02	113.40
1	D	222	ASN	CB-CA-C	17.33	145.05	110.40
1	B	217	GLU	CB-CA-C	16.04	142.49	110.40
1	A	221	ASP	CB-CA-C	-14.65	81.10	110.40
1	C	6	LYS	CB-CA-C	14.12	138.64	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	ASN	CB-CA-C	-14.10	82.20	110.40
1	C	331	LYS	CB-CA-C	13.30	137.01	110.40
1	C	331	LYS	N-CA-CB	-12.98	87.23	110.60
1	D	22	LYS	CB-CA-C	12.81	136.01	110.40
1	C	284	GLU	CA-CB-CG	12.76	141.47	113.40
1	D	214	LEU	CB-CA-C	12.23	133.43	110.20
1	C	14	GLU	N-CA-CB	-11.29	90.27	110.60
1	D	222	ASN	N-CA-CB	-11.21	90.42	110.60
1	B	145	TYR	CB-CG-CD2	11.08	127.65	121.00
1	C	14	GLU	CB-CA-C	-11.02	88.37	110.40
1	A	222	ASN	CA-CB-CG	-10.45	90.40	113.40
1	B	220	THR	N-CA-CB	-10.44	90.47	110.30
1	B	145	TYR	CB-CG-CD1	-10.24	114.85	121.00
1	B	14	GLU	N-CA-CB	10.15	128.88	110.60
1	A	119	PHE	CB-CA-C	-9.62	91.15	110.40
1	B	217	GLU	N-CA-CB	-9.58	93.36	110.60
1	B	14	GLU	CA-CB-CG	9.32	133.91	113.40
1	B	225	GLU	N-CA-CB	-9.12	94.19	110.60
1	B	225	GLU	CB-CA-C	9.08	128.57	110.40
1	D	317	LYS	CB-CA-C	9.07	128.54	110.40
1	A	119	PHE	N-CA-CB	-8.85	94.68	110.60
1	D	229	GLU	CA-CB-CG	-8.84	93.96	113.40
1	B	310	ASP	CB-CG-OD2	8.81	126.23	118.30
1	C	217	GLU	CB-CA-C	8.80	128.00	110.40
1	C	6	LYS	N-CA-CB	-8.71	94.93	110.60
1	D	228	LYS	CA-CB-CG	8.65	132.44	113.40
1	D	229	GLU	CB-CG-CD	-8.60	90.98	114.20
1	D	141	ASP	CB-CG-OD2	8.38	125.84	118.30
1	B	6	LYS	CA-CB-CG	-8.37	95.00	113.40
1	D	82	ASP	CB-CG-OD2	8.12	125.61	118.30
1	C	228	LYS	N-CA-CB	8.01	125.01	110.60
1	D	130	ASP	CB-CG-OD2	7.98	125.48	118.30
1	D	318	LYS	N-CA-CB	7.94	124.89	110.60
1	D	46	ASP	CB-CG-OD2	7.77	125.29	118.30
1	C	229	GLU	CA-CB-CG	-7.72	96.41	113.40
1	B	243	LYS	CB-CA-C	7.64	125.69	110.40
1	C	14	GLU	CA-CB-CG	7.47	129.84	113.40
1	C	155	LYS	N-CA-CB	-7.29	97.49	110.60
1	C	317	LYS	CG-CD-CE	-7.26	90.13	111.90
1	A	141	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	52	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	155	LYS	CB-CA-C	6.95	124.30	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	LYS	CB-CG-CD	6.91	129.56	111.60
1	C	80	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	243	LYS	N-CA-CB	-6.61	98.70	110.60
1	D	221	ASP	CA-CB-CG	6.59	127.90	113.40
1	C	317	LYS	CB-CG-CD	-6.58	94.48	111.60
1	B	325	ASP	CB-CG-OD2	6.55	124.20	118.30
1	D	52	ASP	CB-CG-OD2	6.54	124.18	118.30
1	B	221	ASP	CB-CA-C	6.53	123.45	110.40
1	B	221	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	310	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	6	LYS	CB-CG-CD	-6.44	94.86	111.60
1	D	307	LYS	CA-CB-CG	-6.28	99.59	113.40
1	C	130	ASP	CB-CG-OD2	6.26	123.94	118.30
1	D	284	GLU	N-CA-CB	-6.22	99.40	110.60
1	D	222	ASN	CA-CB-CG	6.20	127.04	113.40
1	A	14	GLU	N-CA-CB	-6.09	99.64	110.60
1	B	155	LYS	N-CA-CB	6.08	121.55	110.60
1	C	223	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	64	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	284	GLU	CA-CB-CG	-6.07	100.05	113.40
1	C	228	LYS	CB-CA-C	6.04	122.47	110.40
1	D	101	GLN	CA-CB-CG	5.93	126.44	113.40
1	D	258	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	101	GLN	CB-CA-C	5.85	122.11	110.40
1	C	284	GLU	CB-CA-C	5.85	122.10	110.40
1	B	220	THR	CA-CB-CG2	5.83	120.56	112.40
1	A	300	LEU	CA-CB-CG	5.81	128.66	115.30
1	D	221	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	56	ASP	CB-CG-OD2	5.67	123.41	118.30
1	D	223	ASP	CB-CG-OD2	5.66	123.39	118.30
1	C	329	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	310	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	228	LYS	CA-CB-CG	5.49	125.47	113.40
1	D	214	LEU	N-CA-CB	-5.47	99.46	110.40
1	B	195	ASP	CB-CG-OD2	5.46	123.22	118.30
1	D	221	ASP	N-CA-CB	-5.44	100.81	110.60
1	D	325	ASP	CB-CG-OD2	5.44	123.19	118.30
1	D	331	LYS	CB-CA-C	-5.40	99.59	110.40
1	A	119	PHE	CA-CB-CG	-5.31	101.15	113.90
1	C	112	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	C	139	PRO	N-CD-CG	-5.30	95.26	103.20
1	B	82	ASP	CB-CG-OD2	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	289	LEU	CA-CB-CG	5.25	127.38	115.30
1	C	166	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	259	LEU	CA-CB-CG	5.17	127.19	115.30
1	D	317	LYS	N-CA-CB	5.16	119.89	110.60
1	A	298	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	14	GLU	CA-CB-CG	5.10	124.61	113.40
1	A	4	LYS	CA-CB-CG	5.08	124.57	113.40
1	B	321	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	217	GLU	CB-CA-C	-5.04	100.32	110.40
1	B	82	ASP	CB-CG-OD1	5.00	122.80	118.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	221	ASP	CA
1	B	222	ASN	CA
1	C	6	LYS	CA
1	C	284	GLU	CA
1	D	221	ASP	CA
1	D	222	ASN	CA
1	D	317	LYS	CA
1	D	318	LYS	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	A	15	GLU	Peptide
1	B	1	ALA	Peptide
1	B	139	PRO	Peptide
1	B	222	ASN	Peptide
1	C	138	ASN	Peptide
1	C	17	THR	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	2555	0	2627	126	4
1	B	2555	0	2627	149	4
1	C	2555	0	2627	113	3
1	D	2555	0	2627	109	3
2	A	44	0	26	1	0
2	B	44	0	26	4	0
2	C	44	0	26	4	0
2	D	44	0	26	4	0
3	A	9	0	0	1	0
3	B	9	0	0	1	0
3	C	9	0	0	3	0
3	D	9	0	0	2	0
4	A	66	0	0	17	0
4	B	76	0	0	34	0
4	C	48	0	0	27	0
4	D	43	0	0	13	0
All	All	10665	0	10612	485	7

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 24.

All (485) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:294:ILE:HB	4:C:452:HOH:O	1.29	1.24
1:B:324:TRP:HB3	4:B:456:HOH:O	1.38	1.23
1:C:152:GLY:HA3	4:C:454:HOH:O	1.42	1.18
1:C:302:SER:HB2	4:C:452:HOH:O	1.49	1.12
1:A:229:GLU:HG3	4:A:456:HOH:O	1.48	1.10
1:C:14:GLU:HA	1:C:15:GLU:HB3	1.25	1.09
1:C:163:CYS:HB2	4:C:435:HOH:O	1.55	1.04
1:B:149:LYS:NZ	1:B:286:GLU:OE1	1.93	1.01
1:A:329:ASP:HB2	4:A:452:HOH:O	1.61	0.98
1:D:75:PRO:HA	4:D:451:HOH:O	1.62	0.98
1:B:306:GLN:HB3	4:B:472:HOH:O	1.64	0.97
1:A:318:LYS:HZ2	1:A:318:LYS:HB3	1.28	0.97
1:A:309:LYS:HG3	4:A:463:HOH:O	1.66	0.93
1:B:327:GLN:HA	1:B:330:LEU:HD22	1.48	0.92
1:C:17:THR:HB	4:C:442:HOH:O	1.70	0.92
1:B:115:ASN:HB3	4:B:451:HOH:O	1.69	0.92
1:B:202:SER:HB2	4:B:469:HOH:O	1.69	0.90
1:C:14:GLU:CA	1:C:15:GLU:HB3	2.04	0.88
1:B:291:LEU:O	1:B:293:CYS:SG	2.33	0.85
1:C:18:VAL:HG22	4:C:424:HOH:O	1.74	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:121:ILE:HD12	1:B:147:THR:HG23	1.58	0.85
1:A:229:GLU:HB3	4:A:455:HOH:O	1.76	0.84
1:A:22:LYS:NZ	1:A:85:VAL:O	2.08	0.84
1:A:166:ASP:HA	4:A:460:HOH:O	1.76	0.84
1:C:152:GLY:CA	4:C:454:HOH:O	2.10	0.84
1:A:318:LYS:NZ	1:A:318:LYS:HB3	1.93	0.83
1:C:217:GLU:O	1:C:220:THR:HG22	1.79	0.83
1:A:329:ASP:C	4:A:452:HOH:O	2.17	0.82
1:C:14:GLU:HA	1:C:15:GLU:CB	2.07	0.82
1:D:196:SER:HB2	1:D:319:SER:OG	1.79	0.82
1:D:138:ASN:HD22	1:D:140:VAL:N	1.79	0.81
1:A:82:ASP:OD1	1:A:84:SER:OG	2.00	0.79
1:A:110:VAL:O	1:A:114:VAL:HG23	1.83	0.79
1:B:113:ASN:O	1:B:116:VAL:HB	1.84	0.78
1:B:138:ASN:ND2	4:B:480:HOH:O	1.94	0.78
1:A:329:ASP:CB	4:A:452:HOH:O	2.21	0.78
1:A:262:SER:OG	1:A:269:ARG:NH2	2.17	0.78
1:A:204:VAL:O	4:A:428:HOH:O	2.01	0.78
1:B:165:LEU:O	1:B:165:LEU:HD12	1.84	0.78
1:B:266:ASN:HD22	1:B:297:ALA:H	1.29	0.77
1:D:281:TYR:CE2	1:D:308:LEU:HD12	2.20	0.76
1:A:223:ASP:O	1:A:224:SER:O	2.03	0.76
1:A:330:LEU:N	4:A:452:HOH:O	2.18	0.76
1:B:201:TRP:HB3	1:B:218:MET:SD	2.27	0.75
1:B:56:ASP:HB2	4:B:452:HOH:O	1.87	0.74
1:B:22:LYS:HZ2	1:B:49:ALA:HB2	1.51	0.74
1:B:229:GLU:OE1	4:B:444:HOH:O	2.06	0.74
1:C:110:VAL:O	1:C:111:GLN:C	2.26	0.73
1:C:19:PRO:O	4:C:424:HOH:O	2.06	0.73
1:C:161:SER:HB2	4:C:427:HOH:O	1.87	0.73
1:D:1:ALA:N	1:D:5:GLU:OE1	2.22	0.73
1:B:111:GLN:O	4:B:417:HOH:O	2.05	0.73
1:B:181:HIS:CE1	4:B:454:HOH:O	2.42	0.73
1:C:121:ILE:HD12	1:C:147:THR:HG23	1.71	0.72
1:A:3:LEU:HD11	1:B:211:LEU:HD13	1.72	0.71
1:A:169:ARG:HD2	4:A:460:HOH:O	1.90	0.71
1:D:100:GLN:NE2	3:D:408:OXQ:O4	2.23	0.70
1:C:21:ASN:HD22	1:C:90:LYS:NZ	1.87	0.70
1:A:127:TYR:CZ	4:A:459:HOH:O	2.44	0.70
1:B:98:VAL:H	1:B:113:ASN:HD21	1.38	0.70
1:B:22:LYS:NZ	1:B:85:VAL:O	2.24	0.70
1:D:222:ASN:HA	4:D:418:HOH:O	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:15:GLU:HB2	4:C:449:HOH:O	1.91	0.70
1:A:147:THR:HG22	1:A:158:VAL:HG11	1.73	0.70
1:B:252:ILE:HD13	2:B:403:NAD:O7N	1.90	0.70
1:D:138:ASN:HD22	1:D:140:VAL:H	1.39	0.70
1:A:21:ASN:ND2	4:A:442:HOH:O	2.25	0.70
1:C:266:ASN:HD22	1:C:297:ALA:H	1.39	0.69
1:D:309:LYS:O	1:D:313:VAL:HG23	1.93	0.69
1:C:294:ILE:O	1:C:294:ILE:HG22	1.91	0.69
1:D:255:SER:O	1:D:256:VAL:C	2.31	0.69
1:D:198:VAL:HG21	1:D:316:LEU:HD13	1.75	0.68
1:D:212:GLN:O	1:D:215:ASN:C	2.32	0.68
1:D:138:ASN:ND2	1:D:140:VAL:H	1.91	0.68
1:B:106:ARG:HB2	4:B:467:HOH:O	1.93	0.68
1:D:17:THR:O	1:D:19:PRO:HD3	1.93	0.67
1:A:30:GLN:NE2	1:A:247:TYR:CZ	2.62	0.67
1:C:290:SER:HB3	4:C:435:HOH:O	1.94	0.67
1:B:296:ASN:ND2	4:B:475:HOH:O	2.29	0.66
1:D:232:LYS:NZ	1:D:236:GLU:OE2	2.16	0.66
1:B:98:VAL:HA	4:B:458:HOH:O	1.95	0.66
1:D:128:SER:N	4:D:434:HOH:O	2.29	0.66
1:C:157:ARG:HD3	4:C:428:HOH:O	1.96	0.66
1:D:135:VAL:HG12	1:D:135:VAL:O	1.96	0.66
1:A:82:ASP:C	1:A:84:SER:H	2.00	0.66
1:B:170:PHE:CD1	1:B:189:ILE:HD11	2.32	0.65
1:A:181:HIS:HD2	1:A:183:SER:H	1.45	0.65
1:C:275:THR:O	1:C:288:PHE:HA	1.98	0.64
1:B:28:VAL:HG23	1:B:28:VAL:O	1.96	0.64
1:B:205:ASN:O	1:B:206:VAL:HG23	1.97	0.64
1:B:113:ASN:O	1:B:116:VAL:N	2.30	0.64
1:C:163:CYS:HA	1:C:166:ASP:OD2	1.98	0.64
1:A:265:LYS:HG3	4:C:450:HOH:O	1.98	0.63
1:A:188:TRP:HZ3	1:A:272:PRO:HD3	1.64	0.63
1:A:49:ALA:C	1:A:50:LEU:HD23	2.18	0.63
1:B:21:ASN:OD1	1:B:90:LYS:NZ	2.30	0.63
1:D:100:GLN:NE2	4:D:419:HOH:O	2.01	0.63
1:C:1:ALA:HB3	1:C:5:GLU:CD	2.20	0.62
1:C:28:VAL:HG11	1:C:50:LEU:HD13	1.82	0.62
1:D:127:TYR:N	4:D:434:HOH:O	2.33	0.62
1:C:17:THR:HA	4:C:442:HOH:O	1.98	0.62
1:A:50:LEU:N	1:A:50:LEU:HD23	2.14	0.62
1:A:111:GLN:HG3	4:A:467:HOH:O	2.00	0.61
2:A:401:NAD:C4N	3:A:402:OXQ:C1	2.78	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:GLN:HB3	4:A:438:HOH:O	2.00	0.61
1:D:241:VAL:HG11	1:D:248:THR:HG22	1.81	0.61
1:B:314:ALA:HA	4:B:440:HOH:O	2.00	0.61
1:B:23:ILE:HD12	1:B:45:ALA:HB2	1.82	0.61
1:D:270:ILE:HA	1:D:293:CYS:O	2.00	0.61
1:B:266:ASN:ND2	1:B:296:ASN:HB2	2.16	0.61
1:B:87:ALA:HA	1:B:127:TYR:O	2.00	0.61
1:A:3:LEU:CD1	1:B:211:LEU:HD13	2.30	0.60
1:B:23:ILE:HD11	1:B:264:LEU:HD11	1.84	0.60
1:D:268:SER:HA	1:D:295:LEU:O	2.00	0.60
1:C:192:GLU:HB3	1:C:196:SER:OG	2.02	0.60
1:C:196:SER:OG	1:C:319:SER:OG	2.19	0.60
1:A:116:VAL:O	1:A:120:ILE:HG23	2.02	0.60
1:A:156:HIS:HB2	1:A:300:LEU:O	2.01	0.60
1:C:290:SER:CB	4:C:435:HOH:O	2.50	0.60
1:D:89:SER:N	1:D:128:SER:OG	2.34	0.59
1:B:61:GLU:OE2	4:B:422:HOH:O	2.15	0.59
1:A:38:SER:O	1:A:42:LYS:HG3	2.02	0.59
1:D:274:SER:HA	1:D:289:LEU:O	2.02	0.59
1:B:44:LEU:HD21	1:B:261:GLU:HG3	1.84	0.59
1:B:50:LEU:HB2	1:B:79:ALA:HB2	1.84	0.59
1:C:242:ILE:HG21	4:C:444:HOH:O	2.03	0.59
1:A:177:LYS:HG2	4:A:451:HOH:O	2.03	0.59
1:C:91:ILE:HD12	1:C:264:LEU:HD21	1.84	0.59
1:C:138:ASN:ND2	3:C:406:OXQ:N5	2.51	0.59
1:A:265:LYS:HE2	4:C:450:HOH:O	2.02	0.59
1:B:45:ALA:O	1:B:74:THR:HG23	2.03	0.59
1:A:42:LYS:HB3	1:A:42:LYS:NZ	2.18	0.58
1:D:153:LEU:O	1:D:154:PRO:C	2.41	0.58
1:C:18:VAL:HG13	1:C:18:VAL:O	2.03	0.58
1:D:110:VAL:HG13	1:D:111:GLN:H	1.68	0.58
1:C:52:ASP:OD2	2:C:405:NAD:O3B	2.13	0.58
1:A:1:ALA:O	1:A:5:GLU:HB2	2.02	0.58
1:B:206:VAL:O	1:B:209:VAL:HG13	2.04	0.58
1:B:223:ASP:HB2	4:B:470:HOH:O	2.03	0.58
1:C:110:VAL:HG13	1:C:111:GLN:N	2.18	0.58
1:B:9:ALA:HB2	1:D:305:ASN:OD1	2.04	0.58
1:B:117:PHE:CE2	1:B:143:LEU:HB3	2.38	0.58
1:C:58:LEU:HG	1:C:79:ALA:HB1	1.84	0.58
1:D:52:ASP:OD2	2:D:407:NAD:O3B	2.19	0.58
1:B:11:VAL:HG23	1:D:303:VAL:HG23	1.86	0.57
1:D:192:GLU:OE1	1:D:196:SER:OG	2.17	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:40:LEU:HD11	1:A:65:LEU:HD13	1.87	0.57
1:C:21:ASN:HD22	1:C:90:LYS:HZ2	1.53	0.57
1:C:136:VAL:HG22	1:C:161:SER:HB3	1.87	0.56
1:A:250:TRP:CZ2	1:B:33:MET:HB3	2.40	0.56
1:D:300:LEU:HD12	1:D:300:LEU:C	2.26	0.56
1:D:27:GLY:O	1:D:32:GLY:HA3	2.05	0.56
1:B:203:GLY:O	1:B:204:VAL:C	2.43	0.56
1:D:201:TRP:HB3	1:D:218:MET:SD	2.46	0.56
1:A:82:ASP:O	1:A:84:SER:N	2.39	0.56
1:B:300:LEU:C	1:B:300:LEU:HD12	2.26	0.56
1:A:28:VAL:O	1:A:57:LYS:NZ	2.37	0.56
1:B:327:GLN:O	1:B:330:LEU:HB2	2.06	0.56
1:D:13:GLU:O	1:D:14:GLU:O	2.24	0.56
1:B:305:ASN:OD1	1:D:9:ALA:HB2	2.06	0.55
1:A:293:CYS:HA	1:A:302:SER:O	2.07	0.55
1:D:140:VAL:O	1:D:144:THR:OG1	2.13	0.55
1:D:106:ARG:NH1	1:D:194:GLY:HA2	2.22	0.55
1:C:255:SER:O	1:C:258:ASP:HB3	2.06	0.55
1:B:294:ILE:HD12	1:B:302:SER:OG	2.06	0.55
1:D:226:ASN:N	1:D:226:ASN:HD22	2.04	0.54
1:C:17:THR:O	1:C:18:VAL:HG12	2.07	0.54
1:B:190:LEU:HD12	1:B:200:VAL:HG21	1.89	0.54
1:C:262:SER:OG	1:C:271:HIS:HE1	1.90	0.54
1:B:100:GLN:CB	4:B:463:HOH:O	2.56	0.54
1:B:149:LYS:HZ1	1:B:286:GLU:CD	2.02	0.54
1:D:17:THR:O	1:D:19:PRO:CD	2.56	0.54
1:A:110:VAL:O	1:A:114:VAL:CG2	2.55	0.54
1:D:132:ILE:HG21	1:D:263:MET:SD	2.47	0.54
1:A:265:LYS:CE	4:C:450:HOH:O	2.55	0.54
1:A:295:LEU:CD2	1:A:300:LEU:HD22	2.38	0.54
1:C:330:LEU:O	1:C:331:LYS:O	2.24	0.54
1:C:169:ARG:O	1:C:173:LEU:HG	2.08	0.54
1:B:303:VAL:HG12	1:B:304:ILE:N	2.23	0.54
1:D:138:ASN:ND2	1:D:140:VAL:N	2.49	0.54
1:C:10:PRO:HD3	4:C:420:HOH:O	2.07	0.54
1:A:252:ILE:O	1:A:256:VAL:HG23	2.08	0.54
1:B:261:GLU:O	1:B:262:SER:C	2.45	0.53
1:B:286:GLU:CG	4:B:460:HOH:O	2.56	0.53
1:D:191:GLY:C	1:D:289:LEU:HD22	2.28	0.53
1:C:259:LEU:O	1:C:263:MET:HG3	2.08	0.53
1:D:314:ALA:O	1:D:317:LYS:N	2.41	0.53
1:B:22:LYS:HG2	1:B:89:SER:HA	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:HIS:CD2	1:A:183:SER:OG	2.62	0.53
1:B:113:ASN:O	1:B:116:VAL:CB	2.56	0.53
1:C:28:VAL:CG1	1:C:50:LEU:HD13	2.37	0.53
1:B:219:GLY:N	4:B:470:HOH:O	2.40	0.53
1:A:204:VAL:HG12	1:A:211:LEU:HD12	1.91	0.53
1:D:196:SER:CB	1:D:319:SER:OG	2.53	0.53
1:B:100:GLN:HB3	4:B:463:HOH:O	2.09	0.53
1:A:130:ASP:HA	1:A:157:ARG:HH12	1.73	0.53
1:A:13:GLU:O	1:A:15:GLU:HB2	2.09	0.53
1:B:271:HIS:O	1:B:273:VAL:N	2.42	0.52
1:A:165:LEU:O	1:A:166:ASP:C	2.46	0.52
1:B:28:VAL:HG23	1:B:57:LYS:HD3	1.91	0.52
1:A:17:THR:O	1:A:18:VAL:HG12	2.10	0.52
1:A:294:ILE:HB	1:A:302:SER:HB2	1.90	0.52
1:B:147:THR:O	1:B:151:SER:OG	2.18	0.52
1:D:196:SER:O	1:D:197:SER:C	2.46	0.52
1:C:327:GLN:HA	1:C:330:LEU:HD22	1.91	0.52
1:C:164:ASN:HD22	1:C:272:PRO:HD2	1.75	0.52
1:A:58:LEU:HD11	1:A:79:ALA:HB1	1.91	0.52
1:D:295:LEU:HA	1:D:299:GLY:O	2.09	0.52
1:A:18:VAL:CG1	1:A:18:VAL:O	2.58	0.52
1:B:306:GLN:CB	4:B:472:HOH:O	2.40	0.51
1:B:69:SER:O	1:B:72:LEU:N	2.39	0.51
1:B:118:LYS:NZ	1:B:331:LYS:O	2.43	0.51
1:C:138:ASN:HD21	3:C:406:OXQ:C1	2.22	0.51
1:A:256:VAL:O	1:A:256:VAL:HG12	2.10	0.51
1:C:181:HIS:CD2	1:C:183:SER:H	2.28	0.51
1:C:296:ASN:ND2	1:C:301:THR:OG1	2.42	0.51
1:B:231:HIS:O	1:B:235:VAL:HG23	2.10	0.51
1:D:205:ASN:ND2	1:D:208:GLY:H	2.08	0.51
1:B:73:GLN:NE2	1:D:261:GLU:OE2	2.39	0.51
1:B:292:PRO:C	1:B:293:CYS:SG	2.89	0.51
1:A:156:HIS:CB	1:A:300:LEU:O	2.58	0.51
1:B:117:PHE:CD2	1:B:143:LEU:HD22	2.45	0.51
1:A:180:ILE:HG22	1:D:294:ILE:HG12	1.93	0.51
1:C:130:ASP:O	1:C:130:ASP:CG	2.48	0.51
1:B:193:HIS:HD2	4:B:480:HOH:O	1.94	0.51
1:A:223:ASP:O	1:A:224:SER:C	2.49	0.51
1:B:24:THR:OG1	1:B:49:ALA:HB3	2.11	0.51
1:C:136:VAL:O	2:C:405:NAD:H2N	2.10	0.51
1:B:164:ASN:HA	1:B:272:PRO:HG2	1.92	0.51
1:C:160:GLY:HA3	1:C:274:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:316:LEU:O	1:B:319:SER:HB2	2.11	0.51
1:B:39:ILE:HD11	1:B:260:ILE:HD13	1.93	0.51
1:B:107:LEU:C	1:B:109:LEU:H	2.14	0.50
1:A:82:ASP:C	1:A:84:SER:N	2.65	0.50
1:B:83:TYR:CE2	1:B:120:ILE:HG23	2.47	0.50
1:B:113:ASN:OD1	1:B:138:ASN:O	2.29	0.50
1:B:83:TYR:CZ	1:B:120:ILE:HG23	2.47	0.50
1:C:18:VAL:O	1:C:18:VAL:CG1	2.60	0.50
1:A:247:TYR:N	1:A:247:TYR:CD2	2.80	0.50
1:B:53:VAL:HG13	2:B:403:NAD:C2A	2.42	0.50
1:A:156:HIS:HB3	1:C:11:VAL:HG12	1.94	0.50
1:B:54:LEU:O	1:B:55:GLU:C	2.50	0.50
1:B:315:GLN:NE2	4:B:474:HOH:O	2.45	0.50
1:C:220:THR:HG23	1:C:220:THR:O	2.12	0.50
1:D:192:GLU:HG3	1:D:323:LEU:HD21	1.92	0.50
1:B:23:ILE:HG22	1:B:24:THR:N	2.26	0.50
1:D:300:LEU:HD12	1:D:300:LEU:O	2.12	0.50
1:C:181:HIS:HD2	1:C:183:SER:HB3	1.77	0.50
1:D:2:THR:HG22	1:D:5:GLU:OE2	2.12	0.49
1:A:147:THR:HG22	1:A:158:VAL:CG1	2.41	0.49
1:B:170:PHE:CG	1:B:189:ILE:HD11	2.46	0.49
1:C:22:LYS:HB3	1:C:89:SER:HA	1.94	0.49
1:D:212:GLN:O	1:D:215:ASN:N	2.45	0.49
1:A:164:ASN:HD22	1:A:272:PRO:HD2	1.76	0.49
1:B:120:ILE:O	1:B:123:GLN:N	2.45	0.49
1:C:240:GLU:HG3	4:C:425:HOH:O	2.12	0.49
1:C:294:ILE:O	1:C:294:ILE:CG2	2.60	0.49
1:C:152:GLY:N	4:C:454:HOH:O	2.35	0.49
1:B:28:VAL:HB	1:B:33:MET:SD	2.52	0.49
1:C:110:VAL:O	1:C:111:GLN:O	2.29	0.49
1:D:274:SER:HA	1:D:290:SER:HA	1.95	0.49
1:B:194:GLY:N	4:B:433:HOH:O	2.44	0.49
1:C:249:ASN:HA	1:C:252:ILE:HG22	1.94	0.49
1:D:18:VAL:HG22	4:D:430:HOH:O	2.13	0.49
1:D:20:ASN:HD22	1:D:20:ASN:C	2.16	0.49
1:D:110:VAL:HG13	1:D:111:GLN:N	2.28	0.49
1:C:156:HIS:HB2	1:C:300:LEU:O	2.13	0.49
1:B:203:GLY:N	4:B:469:HOH:O	2.45	0.49
1:B:215:ASN:ND2	1:B:215:ASN:O	2.46	0.49
1:A:235:VAL:HG12	1:A:236:GLU:N	2.28	0.49
1:D:188:TRP:CH2	1:D:270:ILE:HG22	2.48	0.48
1:B:117:PHE:CG	1:B:143:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:THR:HG21	1:A:86:THR:CG2	2.43	0.48
1:B:252:ILE:HD13	2:B:403:NAD:C7N	2.43	0.48
1:D:315:GLN:HG3	4:D:424:HOH:O	2.13	0.48
1:D:262:SER:OG	1:D:271:HIS:HE1	1.96	0.48
1:A:26:VAL:HG12	1:A:96:ALA:HB2	1.96	0.48
1:B:149:LYS:NZ	4:B:446:HOH:O	2.35	0.48
1:A:30:GLN:NE2	1:A:247:TYR:OH	2.47	0.48
1:B:292:PRO:O	1:B:293:CYS:SG	2.72	0.48
1:D:220:THR:O	1:D:221:ASP:O	2.31	0.48
1:A:31:VAL:HA	1:A:249:ASN:HB2	1.94	0.48
1:D:29:GLY:O	1:D:30:GLN:C	2.51	0.48
1:B:303:VAL:CG1	1:B:304:ILE:N	2.77	0.48
1:B:195:ASP:HA	1:B:235:VAL:HG13	1.95	0.48
1:A:281:TYR:HB3	1:A:313:VAL:HG13	1.95	0.48
1:A:236:GLU:HA	1:A:239:TYR:HD1	1.79	0.48
1:B:277:VAL:HB	1:B:283:ILE:HD13	1.96	0.48
1:A:274:SER:HA	1:A:289:LEU:O	2.14	0.48
1:A:295:LEU:HA	1:A:299:GLY:O	2.13	0.48
1:B:144:THR:O	1:B:147:THR:N	2.45	0.47
1:D:138:ASN:HD22	1:D:139:PRO:HA	1.78	0.47
2:D:407:NAD:C4N	3:D:408:OXQ:C1	2.92	0.47
1:A:269:ARG:HG2	1:D:184:SER:OG	2.14	0.47
1:A:87:ALA:HA	1:A:127:TYR:O	2.14	0.47
1:A:64:ASP:OD2	1:B:245:LYS:NZ	2.45	0.47
1:A:318:LYS:CB	1:A:318:LYS:NZ	2.72	0.47
1:B:2:THR:HG22	1:B:5:GLU:H	1.80	0.47
1:C:252:ILE:HD13	2:C:405:NAD:O7N	2.14	0.47
1:B:23:ILE:CG2	1:B:24:THR:N	2.77	0.47
1:A:13:GLU:O	1:A:14:GLU:C	2.53	0.47
1:D:232:LYS:O	1:D:236:GLU:HG2	2.14	0.47
1:B:259:LEU:HD23	1:B:271:HIS:CD2	2.49	0.47
1:C:164:ASN:ND2	1:C:272:PRO:HD2	2.30	0.47
1:D:2:THR:HG23	1:D:5:GLU:H	1.79	0.47
1:A:86:THR:O	1:A:87:ALA:C	2.54	0.47
2:B:403:NAD:O1A	4:B:424:HOH:O	2.21	0.47
1:D:206:VAL:O	1:D:207:ALA:HB3	2.15	0.46
1:C:110:VAL:O	1:C:114:VAL:HG23	2.15	0.46
1:C:140:VAL:HG21	1:C:161:SER:OG	2.15	0.46
1:A:55:GLU:HG3	1:A:81:LYS:HD3	1.96	0.46
1:B:149:LYS:O	1:B:150:LEU:C	2.53	0.46
1:A:217:GLU:O	1:A:224:SER:CB	2.64	0.46
1:B:15:GLU:O	1:B:16:ALA:HB2	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:191:GLY:HA2	1:C:289:LEU:HD22	1.97	0.46
1:B:241:VAL:HG11	1:B:248:THR:HG22	1.97	0.46
1:D:170:PHE:CD2	1:D:189:ILE:HD11	2.50	0.46
1:C:201:TRP:O	1:C:202:SER:C	2.53	0.46
1:A:83:TYR:O	1:A:127:TYR:CD1	2.69	0.46
1:A:245:LYS:HG3	1:A:247:TYR:O	2.16	0.46
1:A:273:VAL:O	1:A:290:SER:HA	2.15	0.46
1:A:275:THR:O	1:A:277:VAL:HG13	2.16	0.46
1:B:277:VAL:O	1:B:280:MET:HB2	2.15	0.46
1:C:112:ARG:HG3	4:C:445:HOH:O	2.14	0.46
1:A:40:LEU:CD1	1:A:65:LEU:HD13	2.46	0.46
1:C:51:VAL:HG11	1:C:83:TYR:CZ	2.50	0.46
1:A:3:LEU:O	1:A:7:LEU:N	2.48	0.46
1:A:101:GLN:O	1:A:102:GLU:C	2.55	0.46
1:B:324:TRP:CE3	1:B:327:GLN:HB3	2.51	0.45
1:C:157:ARG:CD	4:C:428:HOH:O	2.62	0.45
1:D:291:LEU:O	1:D:293:CYS:SG	2.54	0.45
1:D:26:VAL:HB	1:D:94:VAL:HA	1.97	0.45
1:A:204:VAL:CG1	1:A:211:LEU:HD12	2.46	0.45
1:B:50:LEU:HB2	1:B:79:ALA:CB	2.45	0.45
1:B:288:PHE:O	1:B:289:LEU:HD23	2.16	0.45
1:C:303:VAL:HG12	1:C:304:ILE:N	2.31	0.45
1:A:57:LYS:O	1:A:58:LEU:C	2.55	0.45
1:B:282:GLY:CA	4:B:464:HOH:O	2.64	0.45
1:B:193:HIS:CD2	4:B:480:HOH:O	2.69	0.45
1:A:169:ARG:HG2	1:B:67:HIS:HB3	1.99	0.45
1:D:106:ARG:O	1:D:139:PRO:HD3	2.16	0.45
1:C:21:ASN:HD22	1:C:90:LYS:HZ3	1.62	0.45
1:A:220:THR:O	1:A:222:ASN:N	2.50	0.45
1:C:259:LEU:HD23	1:C:271:HIS:CD2	2.52	0.45
1:B:282:GLY:HA3	4:B:464:HOH:O	2.16	0.45
1:B:275:THR:HA	4:B:466:HOH:O	2.16	0.45
1:D:5:GLU:HB3	4:D:433:HOH:O	2.17	0.45
1:A:130:ASP:HA	1:A:157:ARG:NH1	2.30	0.45
1:C:94:VAL:HG11	1:C:117:PHE:CZ	2.52	0.45
1:A:121:ILE:N	1:A:122:PRO:CD	2.80	0.45
1:A:145:TYR:HB2	1:A:288:PHE:CD2	2.52	0.45
1:B:156:HIS:HB2	1:B:300:LEU:O	2.17	0.45
1:D:136:VAL:O	1:D:137:SER:C	2.55	0.45
1:C:311:ASP:O	1:C:314:ALA:HB3	2.17	0.45
1:A:61:GLU:O	1:A:65:LEU:HG	2.17	0.45
1:B:276:MET:HG2	1:B:288:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:SER:O	1:A:258:ASP:N	2.49	0.45
1:D:190:LEU:HB3	1:D:290:SER:O	2.16	0.44
1:A:106:ARG:NH1	1:A:194:GLY:HA2	2.32	0.44
1:C:294:ILE:HD12	4:C:452:HOH:O	2.17	0.44
1:A:20:ASN:HD21	1:C:21:ASN:HD21	1.65	0.44
1:B:236:GLU:O	1:B:237:SER:C	2.55	0.44
1:C:14:GLU:CA	1:C:15:GLU:CB	2.79	0.44
1:A:244:LEU:HB3	1:B:56:ASP:O	2.17	0.44
1:C:142:ILE:O	1:C:146:VAL:HG23	2.18	0.44
1:D:101:GLN:O	1:D:103:GLY:N	2.51	0.44
1:B:321:ASP:O	1:B:322:THR:C	2.56	0.44
1:D:294:ILE:CD1	1:D:302:SER:OG	2.66	0.44
1:D:154:PRO:HB3	1:D:156:HIS:CE1	2.53	0.44
1:C:160:GLY:HA3	1:C:274:SER:CB	2.47	0.44
1:D:46:ASP:C	1:D:46:ASP:OD1	2.55	0.44
1:C:215:ASN:CG	1:C:215:ASN:O	2.56	0.44
1:A:165:LEU:HD11	1:A:251:ALA:HB1	1.98	0.44
1:D:135:VAL:O	1:D:140:VAL:HG23	2.18	0.44
1:B:87:ALA:O	1:B:88:ASN:C	2.55	0.44
1:C:106:ARG:HG3	4:C:423:HOH:O	2.17	0.44
1:B:203:GLY:O	1:B:205:ASN:N	2.51	0.44
1:C:133:ILE:HG21	1:C:147:THR:HG21	1.98	0.44
1:D:128:SER:C	4:D:434:HOH:O	2.56	0.44
1:B:301:THR:O	1:B:302:SER:HB3	2.18	0.44
1:D:242:ILE:HG22	1:D:243:LYS:N	2.33	0.44
1:A:113:ASN:ND2	1:A:138:ASN:O	2.45	0.44
1:D:125:VAL:C	4:D:434:HOH:O	2.57	0.43
1:C:47:GLU:CD	1:C:76:LYS:HD3	2.39	0.43
1:A:12:ALA:HB2	1:C:156:HIS:CG	2.53	0.43
1:A:218:MET:HE2	1:A:227:TRP:CD2	2.53	0.43
1:D:23:ILE:HD12	1:D:45:ALA:HB2	1.99	0.43
1:B:286:GLU:HG3	4:B:460:HOH:O	2.17	0.43
1:A:235:VAL:HG12	1:A:236:GLU:HG2	2.00	0.43
4:B:455:HOH:O	1:D:15:GLU:HA	2.17	0.43
1:C:110:VAL:CG1	1:C:111:GLN:N	2.81	0.43
1:A:127:TYR:CE1	4:A:459:HOH:O	2.70	0.43
1:A:293:CYS:SG	1:A:300:LEU:HD11	2.59	0.43
1:B:100:GLN:HB3	1:B:104:GLU:HB3	2.01	0.43
1:C:170:PHE:CE1	1:C:174:MET:CE	3.01	0.43
1:D:62:MET:HG2	1:D:66:GLN:NE2	2.33	0.43
1:C:19:PRO:HG3	1:C:47:GLU:OE1	2.18	0.43
1:A:24:THR:HB	1:A:92:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:277:VAL:HG11	1:A:291:LEU:HD11	1.99	0.43
1:D:230:VAL:O	1:D:234:VAL:HG23	2.19	0.43
1:D:247:TYR:HB2	4:D:420:HOH:O	2.18	0.43
1:A:277:VAL:CG1	1:A:291:LEU:HD11	2.49	0.43
1:B:100:GLN:HB2	4:B:463:HOH:O	2.18	0.43
1:D:132:ILE:HD13	1:D:157:ARG:HA	2.01	0.43
1:C:30:GLN:CD	1:C:247:TYR:CZ	2.92	0.43
1:C:222:ASN:O	1:C:223:ASP:O	2.37	0.43
1:B:106:ARG:HD3	1:B:138:ASN:ND2	2.33	0.42
1:C:215:ASN:O	1:C:218:MET:HB3	2.18	0.42
1:D:120:ILE:O	1:D:123:GLN:HB2	2.18	0.42
1:D:69:SER:HB3	4:D:445:HOH:O	2.18	0.42
1:C:22:LYS:C	1:C:23:ILE:HG13	2.39	0.42
1:C:265:LYS:HD3	4:C:408:HOH:O	2.18	0.42
1:D:300:LEU:C	1:D:300:LEU:CD1	2.87	0.42
1:A:20:ASN:HD21	1:C:21:ASN:ND2	2.18	0.42
1:A:50:LEU:N	1:A:50:LEU:CD2	2.82	0.42
1:B:69:SER:O	1:B:71:PHE:N	2.53	0.42
1:D:170:PHE:CG	1:D:189:ILE:HD11	2.54	0.42
1:A:28:VAL:HG12	1:A:50:LEU:HD13	2.02	0.42
1:A:65:LEU:O	1:A:66:GLN:C	2.58	0.42
1:B:2:THR:HG22	1:B:5:GLU:N	2.34	0.42
1:B:115:ASN:HB2	4:B:417:HOH:O	2.19	0.42
1:B:165:LEU:HD12	1:B:165:LEU:C	2.40	0.42
1:C:153:LEU:HD22	1:C:157:ARG:HH12	1.83	0.42
1:C:1:ALA:HB3	1:C:5:GLU:CG	2.49	0.42
1:B:174:MET:SD	1:B:185:CYS:HB3	2.60	0.42
1:B:266:ASN:CG	1:B:266:ASN:O	2.56	0.42
1:D:153:LEU:C	1:D:154:PRO:O	2.56	0.42
1:B:300:LEU:CD1	1:B:300:LEU:C	2.88	0.42
1:B:2:THR:HG22	1:B:5:GLU:HB2	2.01	0.42
1:B:12:ALA:HB1	1:D:298:ARG:NH2	2.35	0.42
1:B:119:PHE:C	1:B:119:PHE:CD1	2.91	0.42
1:A:273:VAL:HG23	1:A:300:LEU:CD2	2.50	0.42
1:C:255:SER:O	1:C:258:ASP:CB	2.68	0.42
1:B:321:ASP:O	1:B:324:TRP:N	2.53	0.42
1:D:2:THR:HG22	1:D:5:GLU:CD	2.40	0.42
1:A:141:ASP:HB3	1:A:288:PHE:O	2.19	0.42
1:B:126:LYS:HD3	1:B:127:TYR:CE1	2.54	0.42
1:B:83:TYR:OH	1:B:120:ILE:HG12	2.20	0.42
1:D:2:THR:HG22	1:D:5:GLU:CG	2.50	0.41
1:C:177:LYS:HE2	1:C:226:ASN:ND2	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:294:ILE:HD12	1:D:302:SER:OG	2.19	0.41
1:D:166:ASP:OD2	1:D:193:HIS:CE1	2.73	0.41
1:C:220:THR:CG2	1:C:220:THR:O	2.68	0.41
1:B:274:SER:HA	1:B:290:SER:HA	2.01	0.41
1:D:301:THR:O	1:D:302:SER:HB3	2.20	0.41
1:A:263:MET:HA	1:A:296:ASN:O	2.20	0.41
1:B:142:ILE:HG13	1:B:323:LEU:CD1	2.51	0.41
1:D:260:ILE:HG22	1:D:264:LEU:HD12	2.03	0.41
1:D:65:LEU:O	1:D:66:GLN:C	2.57	0.41
1:A:56:ASP:OD1	4:A:404:HOH:O	2.21	0.41
1:A:329:ASP:O	1:A:330:LEU:C	2.58	0.41
2:D:407:NAD:H3B	4:D:443:HOH:O	2.21	0.41
1:B:156:HIS:CD2	1:B:157:ARG:HG2	2.55	0.41
1:D:260:ILE:CG2	1:D:264:LEU:HD12	2.51	0.41
1:C:118:LYS:HE2	1:C:332:PHE:HB3	2.01	0.41
1:B:149:LYS:CE	1:B:286:GLU:OE1	2.68	0.41
1:B:110:VAL:HG22	1:B:111:GLN:N	2.35	0.41
1:B:121:ILE:HB	1:B:122:PRO:HD3	2.03	0.41
1:D:18:VAL:HA	1:D:19:PRO:HD2	1.76	0.41
1:C:164:ASN:HA	1:C:164:ASN:HD22	1.78	0.41
1:C:225:GLU:O	1:C:226:ASN:CG	2.58	0.41
1:C:109:LEU:HB2	1:C:139:PRO:HD2	2.03	0.41
1:B:106:ARG:O	1:B:109:LEU:HD12	2.21	0.41
1:B:138:ASN:OD1	3:B:404:OXQ:N5	2.54	0.41
1:B:199:ALA:O	1:B:201:TRP:N	2.54	0.41
1:D:2:THR:O	1:D:5:GLU:N	2.54	0.41
1:A:292:PRO:HB2	1:A:304:ILE:HB	2.03	0.41
1:A:294:ILE:HD11	1:A:304:ILE:HD11	2.03	0.41
1:C:55:GLU:CG	1:C:81:LYS:HD3	2.51	0.41
1:B:206:VAL:O	1:B:209:VAL:CG1	2.69	0.40
1:D:197:SER:HB2	1:D:231:HIS:HE1	1.85	0.40
1:D:96:ALA:HB1	2:D:407:NAD:C4A	2.51	0.40
1:C:240:GLU:CG	4:C:425:HOH:O	2.69	0.40
1:C:118:LYS:NZ	1:C:332:PHE:HB3	2.35	0.40
1:D:197:SER:O	1:D:231:HIS:NE2	2.53	0.40
1:A:28:VAL:HG22	1:A:52:ASP:OD2	2.21	0.40
1:A:270:ILE:HA	1:A:293:CYS:O	2.22	0.40
1:D:57:LYS:NZ	1:D:61:GLU:OE2	2.53	0.40
1:A:24:THR:CG2	1:A:86:THR:HG22	2.51	0.40
1:D:241:VAL:CG1	1:D:248:THR:HG22	2.48	0.40
1:C:18:VAL:O	1:C:19:PRO:C	2.60	0.40
1:A:29:GLY:O	1:A:30:GLN:C	2.60	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:144:THR:HG22	1:C:288:PHE:CD1	2.57	0.40
1:C:188:TRP:CD1	1:C:188:TRP:N	2.89	0.40
2:C:405:NAD:C5N	3:C:406:OXQ:N3	2.85	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	Distance(Å)	Clash(Å)
1:A:149:LYS:CA	1:B:14:GLU:OE2[1_554]	1.19	1.01
1:C:14:GLU:OE1	1:D:149:LYS:NZ[1_554]	1.69	0.51
1:A:148:TRP:O	1:B:14:GLU:OE1[1_554]	1.75	0.45
1:A:149:LYS:C	1:B:14:GLU:OE2[1_554]	1.78	0.42
1:C:14:GLU:OE2	1:D:149:LYS:NZ[1_554]	1.82	0.38
1:C:14:GLU:CD	1:D:149:LYS:NZ[1_554]	1.94	0.26
1:A:149:LYS:O	1:B:14:GLU:OE2[1_554]	2.02	0.18

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	330/333 (99%)	272 (82%)	45 (14%)	13 (4%)	5	26
1	B	330/333 (99%)	264 (80%)	51 (16%)	15 (4%)	4	22
1	C	330/333 (99%)	275 (83%)	45 (14%)	10 (3%)	7	34
1	D	330/333 (99%)	269 (82%)	49 (15%)	12 (4%)	5	29
All	All	1320/1332 (99%)	1080 (82%)	190 (14%)	50 (4%)	5	27

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	221	ASP
1	A	222	ASN
1	A	224	SER
1	A	226	ASN

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Mol	Chain	Res	Type
1	B	16	ALA
1	B	70	LEU
1	B	110	VAL
1	B	197	SER
1	B	237	SER
1	C	15	GLU
1	C	139	PRO
1	C	331	LYS
1	D	14	GLU
1	D	204	VAL
1	D	221	ASP
1	A	13	GLU
1	A	20	ASN
1	A	331	LYS
1	B	2	THR
1	B	55	GLU
1	B	204	VAL
1	B	213	GLU
1	C	223	ASP
1	D	194	GLY
1	A	193	HIS
1	B	14	GLU
1	B	221	ASP
1	C	104	GLU
1	D	13	GLU
1	D	102	GLU
1	D	200	VAL
1	A	17	THR
1	A	18	VAL
1	A	102	GLU
1	B	144	THR
1	C	226	ASN
1	A	83	TYR
1	B	331	LYS
1	C	18	VAL
1	C	19	PRO
1	C	222	ASN
1	C	249	ASN
1	D	16	ALA
1	D	28	VAL
1	D	18	VAL
1	D	110	VAL

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Mol	Chain	Res	Type
1	B	182	PRO
1	B	206	VAL
1	D	256	VAL

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	288/289 (100%)	236 (82%)	52 (18%)	2	13
1	B	288/289 (100%)	248 (86%)	40 (14%)	5	23
1	C	288/289 (100%)	241 (84%)	47 (16%)	3	17
1	D	288/289 (100%)	241 (84%)	47 (16%)	3	17
All	All	1152/1156 (100%)	966 (84%)	186 (16%)	3	17

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LEU
1	A	5	GLU
1	A	6	LYS
1	A	7	LEU
1	A	11	VAL
1	A	14	GLU
1	A	15	GLU
1	A	18	VAL
1	A	21	ASN
1	A	50	LEU
1	A	55	GLU
1	A	57	LYS
1	A	81	LYS
1	A	84	SER
1	A	106	ARG
1	A	108	ASN
1	A	111	GLN
1	A	120	ILE

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Mol	Chain	Res	Type
1	A	128	SER
1	A	147	THR
1	A	158	VAL
1	A	182	PRO
1	A	202	SER
1	A	205	ASN
1	A	214	LEU
1	A	217	GLU
1	A	220	THR
1	A	221	ASP
1	A	222	ASN
1	A	223	ASP
1	A	224	SER
1	A	228	LYS
1	A	235	VAL
1	A	244	LEU
1	A	266	ASN
1	A	273	VAL
1	A	274	SER
1	A	275	THR
1	A	276	MET
1	A	290	SER
1	A	300	LEU
1	A	303	VAL
1	A	307	LYS
1	A	311	ASP
1	A	315	GLN
1	A	317	LYS
1	A	318	LYS
1	A	323	LEU
1	A	325	ASP
1	A	330	LEU
1	A	332	PHE
1	B	2	THR
1	B	3	LEU
1	B	17	THR
1	B	20	ASN
1	B	33	MET
1	B	51	VAL
1	B	56	ASP
1	B	81	LYS
1	B	88	ASN

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Mol	Chain	Res	Type
1	B	107	LEU
1	B	108	ASN
1	B	110	VAL
1	B	111	GLN
1	B	128	SER
1	B	131	CYS
1	B	137	SER
1	B	141	ASP
1	B	157	ARG
1	B	176	GLU
1	B	197	SER
1	B	209	VAL
1	B	214	LEU
1	B	224	SER
1	B	228	LYS
1	B	231	HIS
1	B	232	LYS
1	B	262	SER
1	B	277	VAL
1	B	278	LYS
1	B	283	ILE
1	B	287	VAL
1	B	289	LEU
1	B	295	LEU
1	B	300	LEU
1	B	310	ASP
1	B	315	GLN
1	B	317	LYS
1	B	322	THR
1	B	323	LEU
1	B	330	LEU
1	C	6	LYS
1	C	7	LEU
1	C	11	VAL
1	C	13	GLU
1	C	14	GLU
1	C	15	GLU
1	C	17	THR
1	C	21	ASN
1	C	46	ASP
1	C	57	LYS
1	C	62	MET

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Mol	Chain	Res	Type
1	C	80	ASP
1	C	81	LYS
1	C	89	SER
1	C	111	GLN
1	C	115	ASN
1	C	128	SER
1	C	141	ASP
1	C	142	ILE
1	C	155	LYS
1	C	157	ARG
1	C	161	SER
1	C	164	ASN
1	C	177	LYS
1	C	202	SER
1	C	214	LEU
1	C	215	ASN
1	C	225	GLU
1	C	229	GLU
1	C	233	MET
1	C	237	SER
1	C	243	LYS
1	C	245	LYS
1	C	248	THR
1	C	262	SER
1	C	268	SER
1	C	274	SER
1	C	276	MET
1	C	281	TYR
1	C	285	ASN
1	C	289	LEU
1	C	300	LEU
1	C	317	LYS
1	C	319	SER
1	C	323	LEU
1	C	330	LEU
1	C	331	LYS
1	D	3	LEU
1	D	14	GLU
1	D	17	THR
1	D	18	VAL
1	D	20	ASN
1	D	38	SER

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Mol	Chain	Res	Type
1	D	81	LYS
1	D	98	VAL
1	D	107	LEU
1	D	119	PHE
1	D	130	ASP
1	D	138	ASN
1	D	147	THR
1	D	166	ASP
1	D	174	MET
1	D	177	LYS
1	D	195	ASP
1	D	196	SER
1	D	197	SER
1	D	202	SER
1	D	205	ASN
1	D	209	VAL
1	D	221	ASP
1	D	223	ASP
1	D	226	ASN
1	D	228	LYS
1	D	229	GLU
1	D	232	LYS
1	D	233	MET
1	D	237	SER
1	D	242	ILE
1	D	255	SER
1	D	261	GLU
1	D	274	SER
1	D	285	ASN
1	D	289	LEU
1	D	290	SER
1	D	300	LEU
1	D	310	ASP
1	D	311	ASP
1	D	315	GLN
1	D	316	LEU
1	D	317	LYS
1	D	319	SER
1	D	322	THR
1	D	326	ILE
1	D	331	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	30	GLN
1	A	108	ASN
1	A	164	ASN
1	A	181	HIS
1	A	205	ASN
1	A	231	HIS
1	A	266	ASN
1	B	20	ASN
1	B	113	ASN
1	B	156	HIS
1	B	164	ASN
1	B	181	HIS
1	B	212	GLN
1	B	266	ASN
1	B	271	HIS
1	B	306	GLN
1	B	315	GLN
1	C	21	ASN
1	C	108	ASN
1	C	115	ASN
1	C	181	HIS
1	C	205	ASN
1	C	212	GLN
1	C	266	ASN
1	C	271	HIS
1	C	327	GLN
1	D	20	ASN
1	D	66	GLN
1	D	113	ASN
1	D	138	ASN
1	D	156	HIS
1	D	181	HIS
1	D	186	HIS
1	D	205	ASN
1	D	226	ASN
1	D	266	ASN
1	D	271	HIS
1	D	315	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 ⓘ

8 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	401	-	48,48,48	1.61	5 (10%)	73,73,73	2.03	16 (21%)
3	OXQ	A	402	-	7,9,9	1.93	3 (42%)	6,12,12	1.68	2 (33%)
2	NAD	B	403	-	48,48,48	1.66	3 (6%)	73,73,73	2.73	18 (24%)
3	OXQ	B	404	-	7,9,9	2.26	3 (42%)	6,12,12	1.95	2 (33%)
2	NAD	C	405	-	48,48,48	1.58	7 (14%)	73,73,73	2.17	12 (16%)
3	OXQ	C	406	-	7,9,9	1.88	2 (28%)	6,12,12	0.99	0
2	NAD	D	407	-	48,48,48	1.71	5 (10%)	73,73,73	2.06	14 (19%)
3	OXQ	D	408	-	7,9,9	2.16	4 (57%)	6,12,12	2.30	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	NAD	A	401	-	-	0/30/62/62	0/3/5/5
3	OXQ	A	402	-	-	1/3/4/4	0/0/1/1
2	NAD	B	403	-	-	0/30/62/62	0/3/5/5
3	OXQ	B	404	-	-	1/3/4/4	0/0/1/1
2	NAD	C	405	-	-	0/30/62/62	0/3/5/5
3	OXQ	C	406	-	-	1/3/4/4	0/0/1/1
2	NAD	D	407	-	-	0/30/62/62	0/3/5/5
3	OXQ	D	408	-	-	1/3/4/4	0/0/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	403	NAD	O7N-C7N	8.36	1.43	1.24
2	D	407	NAD	O7N-C7N	7.99	1.42	1.24
2	A	401	NAD	O7N-C7N	7.52	1.41	1.24
2	C	405	NAD	O7N-C7N	5.94	1.38	1.24
2	D	407	NAD	C2A-N3A	5.09	1.42	1.32
2	A	401	NAD	C2A-N3A	4.29	1.40	1.32
3	B	404	OXQ	C1-N5	3.68	1.34	1.31
2	D	407	NAD	C2A-N1A	3.66	1.41	1.33
3	C	406	OXQ	C2-N3	-3.62	1.31	1.38
3	B	404	OXQ	C2-N3	-3.54	1.31	1.38
3	A	402	OXQ	C2-N3	-3.50	1.31	1.38
3	D	408	OXQ	C2-N3	-3.23	1.32	1.38
2	C	405	NAD	C2D-C1D	-3.21	1.48	1.53
2	C	405	NAD	C2A-N3A	3.17	1.38	1.32
2	A	401	NAD	C2A-N1A	3.11	1.40	1.33
2	C	405	NAD	C2A-N1A	3.06	1.39	1.33
3	B	404	OXQ	O9-C6	-2.99	1.21	1.30
2	A	401	NAD	C2D-C1D	-2.85	1.49	1.53
2	B	403	NAD	C2A-N1A	2.84	1.39	1.33
2	B	403	NAD	C2A-N3A	2.74	1.37	1.32
3	C	406	OXQ	O9-C6	-2.70	1.21	1.30
3	D	408	OXQ	C2-C6	-2.63	1.47	1.51
2	C	405	NAD	C4A-N9A	-2.61	1.33	1.37
3	D	408	OXQ	O9-C6	-2.57	1.22	1.30
3	D	408	OXQ	C1-N5	2.33	1.33	1.31
2	C	405	NAD	O4B-C1B	-2.32	1.37	1.41
2	D	407	NAD	C2N-N1N	2.32	1.38	1.35
3	A	402	OXQ	C1-N5	2.29	1.33	1.31
2	A	401	NAD	O4D-C4D	-2.23	1.39	1.45
2	D	407	NAD	C2N-C3N	2.22	1.42	1.38
3	A	402	OXQ	O9-C6	-2.21	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	405	NAD	C2B-C1B	-2.06	1.50	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	NAD	N3A-C2A-N1A	-14.48	116.60	128.71
2	B	403	NAD	O4B-C1B-N9A	10.08	117.81	108.44
2	C	405	NAD	N3A-C2A-N1A	-8.94	121.23	128.71
2	D	407	NAD	O4B-C1B-N9A	8.85	116.67	108.44
2	A	401	NAD	N3A-C2A-N1A	-8.38	121.70	128.71
2	D	407	NAD	N3A-C2A-N1A	-7.53	122.42	128.71
2	A	401	NAD	O4D-C1D-N1N	7.47	115.59	107.95
2	B	403	NAD	O4D-C1D-N1N	6.40	114.50	107.95
2	C	405	NAD	C1B-N9A-C4A	-5.86	116.51	126.64
2	C	405	NAD	C3N-C7N-N7N	5.47	123.99	117.77
2	C	405	NAD	O7N-C7N-N7N	-5.01	115.36	122.59
2	C	405	NAD	O4D-C1D-N1N	4.83	112.90	107.95
2	D	407	NAD	C4B-O4B-C1B	-4.78	104.55	109.75
2	B	403	NAD	C1B-N9A-C4A	-4.67	118.57	126.64
2	D	407	NAD	N3A-C4A-N9A	4.54	133.63	125.43
2	B	403	NAD	O7N-C7N-C3N	4.36	124.49	119.58
2	C	405	NAD	O4B-C1B-N9A	4.27	112.41	108.44
2	B	403	NAD	O7N-C7N-N7N	-4.23	116.48	122.59
2	C	405	NAD	C8A-N9A-C1B	3.99	134.24	126.38
2	A	401	NAD	N3A-C4A-N9A	3.93	132.52	125.43
2	D	407	NAD	PN-O3-PA	-3.81	116.60	132.95
2	A	401	NAD	C4D-O4D-C1D	-3.79	105.63	109.75
2	C	405	NAD	PN-O3-PA	-3.67	117.19	132.95
2	D	407	NAD	O4B-C1B-C2B	-3.65	101.17	106.77
2	A	401	NAD	O4B-C1B-N9A	3.62	111.80	108.44
3	D	408	OXQ	C1-C2-C6	-3.62	123.84	130.79
2	B	403	NAD	O3D-C3D-C4D	-3.54	100.65	111.08
2	B	403	NAD	PN-O3-PA	-3.36	118.54	132.95
3	B	404	OXQ	O8-C6-C2	3.33	127.23	121.04
2	C	405	NAD	C4A-C5A-N7A	-3.17	106.81	109.52
2	A	401	NAD	O2N-PN-O1N	3.13	128.16	118.72
2	A	401	NAD	O4D-C1D-C2D	-3.12	101.99	106.77
2	D	407	NAD	O4D-C1D-C2D	-3.07	102.06	106.77
2	B	403	NAD	C8A-N9A-C1B	3.06	132.41	126.38
2	C	405	NAD	C8A-N9A-C4A	3.04	109.22	106.90
3	D	408	OXQ	O7-C1-C2	-3.01	125.12	128.67
3	B	404	OXQ	O9-C6-O8	-2.97	116.60	123.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAD	O4B-C1B-C2B	-2.92	102.30	106.77
2	A	401	NAD	C5A-C4A-N3A	-2.89	119.40	125.70
2	B	403	NAD	O3B-C3B-C2B	-2.85	102.56	111.83
2	A	401	NAD	C3D-C2D-C1D	-2.75	96.60	100.91
2	D	407	NAD	C2D-C1D-N1N	2.63	118.31	113.86
2	A	401	NAD	C3B-C2B-C1B	2.62	105.01	100.91
2	C	405	NAD	N7A-C8A-N9A	-2.61	106.98	114.36
2	A	401	NAD	PN-O3-PA	-2.61	121.74	132.95
2	D	407	NAD	C5A-C4A-N3A	-2.60	120.04	125.70
2	D	407	NAD	C6A-C5A-C4A	2.55	121.93	117.25
2	B	403	NAD	C8A-N9A-C4A	2.50	108.81	106.90
2	D	407	NAD	C3B-C2B-C1B	-2.47	97.03	100.91
2	B	403	NAD	N3A-C4A-N9A	2.47	129.89	125.43
3	A	402	OXQ	O7-C1-C2	-2.47	125.75	128.67
3	A	402	OXQ	C1-C2-C6	-2.37	126.24	130.79
2	A	401	NAD	C6A-C5A-C4A	2.35	121.55	117.25
2	A	401	NAD	O3D-C3D-C2D	-2.34	104.23	111.83
2	B	403	NAD	C2B-C1B-N9A	-2.31	107.33	113.27
2	B	403	NAD	C3D-C2D-C1D	-2.31	97.30	100.91
2	A	401	NAD	O3-PN-O1N	-2.30	103.34	108.83
2	B	403	NAD	C2A-N1A-C6A	2.28	122.89	118.77
2	D	407	NAD	C3N-C7N-N7N	2.28	120.37	117.77
2	B	403	NAD	N7A-C8A-N9A	-2.23	108.04	114.36
2	D	407	NAD	O2B-C2B-C3B	2.23	119.08	111.83
2	A	401	NAD	O2B-C2B-C3B	-2.18	104.75	111.83
2	C	405	NAD	O2N-PN-O1N	2.12	125.10	118.72
2	D	407	NAD	N7A-C8A-N9A	-2.11	108.39	114.36
2	B	403	NAD	C2A-N3A-C4A	2.08	119.94	114.01
2	B	403	NAD	O2D-C2D-C3D	2.06	118.55	111.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	404	OXQ	O9-C6-C2-C1
3	C	406	OXQ	O9-C6-C2-C1
3	A	402	OXQ	O9-C6-C2-C1
3	D	408	OXQ	O9-C6-C2-C1

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	332/333 (99%)	-0.46	0 100 100	37, 50, 82, 93	11 (3%)
1	B	332/333 (99%)	-0.36	0 100 100	38, 61, 85, 90	15 (4%)
1	C	332/333 (99%)	-0.44	0 100 100	37, 54, 84, 92	14 (4%)
1	D	332/333 (99%)	-0.44	0 100 100	37, 53, 85, 93	18 (5%)
All	All	1328/1332 (99%)	-0.42	0 100 100	37, 54, 84, 93	58 (4%)

There are no RSRZ outliers to report.

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
3	OXQ	A	402	9/9	0.16	1.02	63,64,65,65	0
3	OXQ	D	408	9/9	0.17	0.81	63,65,67,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	OXQ	C	406	9/9	0.17	0.70	56,58,59,59	0
3	OXQ	B	404	9/9	0.18	0.33	53,56,60,62	0
2	NAD	A	401	44/44	0.14	0.12	29,40,50,51	0
2	NAD	C	405	44/44	0.14	-0.38	33,43,52,57	0
2	NAD	B	403	44/44	0.16	-0.40	46,61,84,87	0
2	NAD	D	407	44/44	0.12	-0.93	33,42,47,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.