



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:09 PM UTC

PDB ID : 1NIS / pdb_00001nis
Title : CRYSTAL STRUCTURE OF ACONITASE WITH TRANS-ACONITATE
AND NITROCITRATE BOUND
Authors : Lauble, H.; Kennedy, M.C.; Beinert, H.; Stout, C.D.
Deposited on : 1993-01-17
Resolution : 2.05 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

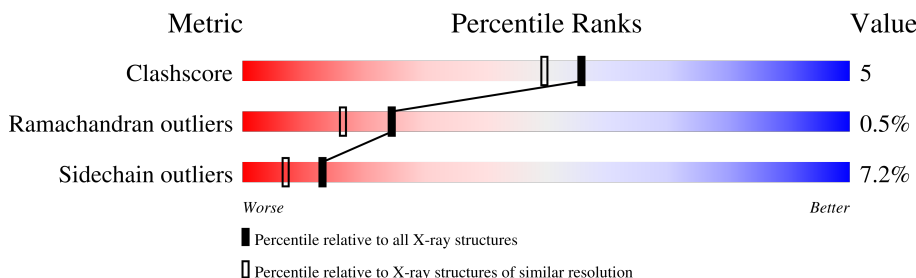
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	754	 75% 19% . .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6130 atoms, of which 7 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ACONITASE.

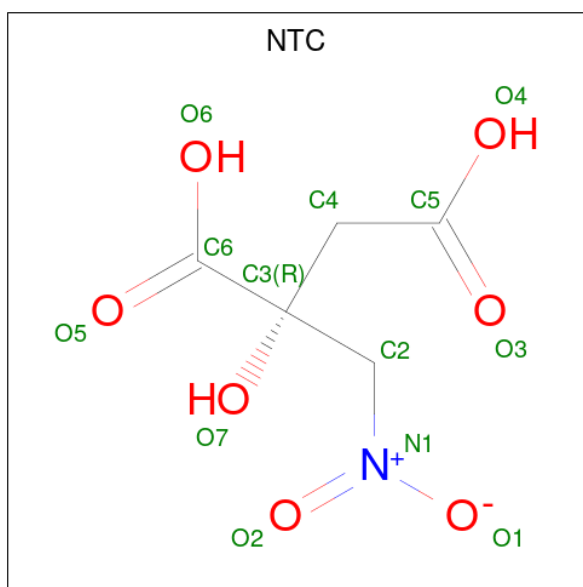
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	753	5812	3664	1031	1095	22	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0

- Molecule 3 is 2-HYDROXY-2-NITROMETHYL SUCCINIC ACID (CCD ID: NTC) (formula: $\text{C}_5\text{H}_7\text{NO}_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			18	5	5	1	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	290	Total	H	O	0	0
			292	2	290		

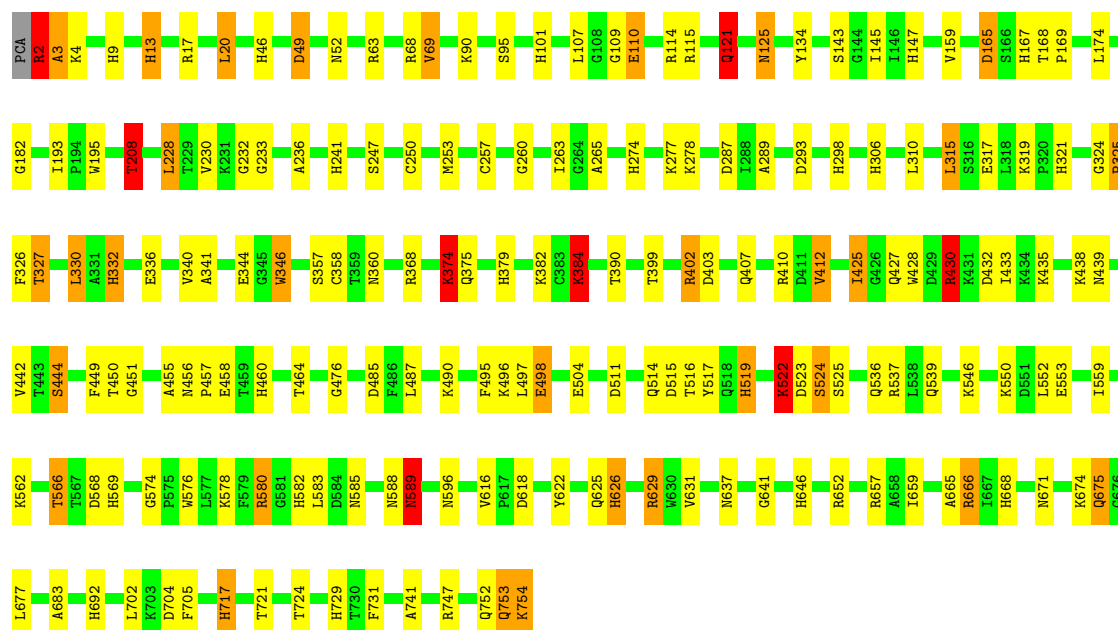
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

• Molecule 1: ACONITASE

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	185.50Å 72.00Å 73.00Å 90.00° 90.00° 77.70°	Depositor
Resolution (Å)	8.00 – 2.05	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.05)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6130	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

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: SF4, NTC

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	1.08	29/5938 (0.5%)	1.78	128/8044 (1.6%)

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	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	626	HIS	CD2-NE2	-7.29	1.29	1.37
1	A	13	HIS	CD2-NE2	-7.15	1.29	1.37
1	A	519	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	321	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	717	HIS	CD2-NE2	-6.76	1.30	1.37
1	A	582	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	101	HIS	CD2-NE2	-6.59	1.30	1.37
1	A	298	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	332	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	460	HIS	CD2-NE2	-6.09	1.31	1.37
1	A	379	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	167	HIS	CD2-NE2	-5.95	1.31	1.37
1	A	306	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	646	HIS	CD2-NE2	-5.81	1.31	1.37
1	A	9	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	580	ARG	CD-NE	-5.78	1.38	1.46
1	A	692	HIS	CD2-NE2	-5.64	1.31	1.37
1	A	569	HIS	CD2-NE2	-5.63	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	VAL	CA-CB	5.60	1.60	1.54
1	A	729	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	46	HIS	CD2-NE2	-5.53	1.31	1.37
1	A	147	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	559	ILE	CA-CB	5.47	1.61	1.54
1	A	616	VAL	CA-CB	5.46	1.57	1.54
1	A	626	HIS	CG-ND1	-5.20	1.32	1.38
1	A	241	HIS	CD2-NE2	-5.16	1.32	1.37
1	A	668	HIS	CD2-NE2	-5.11	1.32	1.37
1	A	425	ILE	CA-CB	5.08	1.61	1.54
1	A	629	ARG	NE-CZ	5.02	1.38	1.33

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	580	ARG	NE-CZ-NH2	-10.47	109.78	119.20
1	A	402	ARG	NE-CZ-NH2	-9.84	110.34	119.20
1	A	63	ARG	NE-CZ-NH2	-7.79	112.18	119.20
1	A	498	GLU	CA-CB-CG	7.74	129.58	114.10
1	A	3	ALA	N-CA-C	-7.50	100.42	110.55
1	A	274	HIS	CB-CG-CD2	-7.49	121.46	131.20
1	A	666	ARG	NE-CZ-NH2	-7.31	112.62	119.20
1	A	430	ARG	NE-CZ-NH2	-7.27	112.66	119.20
1	A	566	THR	N-CA-CB	-7.23	100.47	110.38
1	A	729	HIS	CB-CG-CD2	-7.16	121.89	131.20
1	A	582	HIS	CB-CG-CD2	-7.12	121.94	131.20
1	A	539	GLN	CG-CD-NE2	7.10	127.04	116.40
1	A	515	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	9	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	637	ASN	OD1-CG-ND2	-6.95	115.65	122.60
1	A	101	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	A	46	HIS	CB-CG-CD2	-6.88	122.26	131.20
1	A	410	ARG	NE-CZ-NH2	-6.84	113.05	119.20
1	A	731	PHE	CA-CB-CG	6.79	120.58	113.80
1	A	522	LYS	CG-CD-CE	6.75	126.83	111.30
1	A	705	PHE	CA-CB-CG	6.75	120.55	113.80
1	A	412	VAL	CB-CA-C	-6.67	100.34	111.29
1	A	522	LYS	O-C-N	6.67	130.34	122.34
1	A	717	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	A	511	ASP	N-CA-C	-6.55	99.09	109.04
1	A	449	PHE	CA-CB-CG	6.53	120.33	113.80
1	A	460	HIS	CB-CG-CD2	-6.53	122.71	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	THR	N-CA-CB	-6.47	100.28	111.55
1	A	495	PHE	CA-CB-CG	6.44	120.24	113.80
1	A	427	GLN	OE1-CD-NE2	-6.39	116.21	122.60
1	A	589	ASN	OD1-CG-ND2	-6.38	116.22	122.60
1	A	321	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	A	274	HIS	CB-CG-ND1	6.33	132.20	122.70
1	A	659	ILE	N-CA-C	-6.33	98.40	107.77
1	A	519	HIS	CB-CG-ND1	6.32	132.18	122.70
1	A	384	LYS	N-CA-C	-6.31	103.68	112.45
1	A	13	HIS	CB-CG-CD2	-6.25	123.07	131.20
1	A	519	HIS	CB-CG-CD2	-6.14	123.21	131.20
1	A	753	GLN	N-CA-C	6.14	123.89	110.80
1	A	101	HIS	CB-CG-ND1	6.14	131.91	122.70
1	A	569	HIS	CB-CG-ND1	6.13	131.90	122.70
1	A	298	HIS	CB-CG-CD2	-6.10	123.27	131.20
1	A	374	LYS	CA-CB-CG	6.07	126.23	114.10
1	A	588	ASN	OD1-CG-ND2	-6.04	116.56	122.60
1	A	569	HIS	CB-CG-CD2	-6.02	123.38	131.20
1	A	485	ASP	N-CA-C	6.01	118.67	110.55
1	A	668	HIS	CA-CB-CG	-6.01	107.79	113.80
1	A	692	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	580	ARG	CG-CD-NE	-5.90	99.02	112.00
1	A	69	VAL	O-C-N	-5.87	116.84	123.18
1	A	683	ALA	N-CA-C	-5.85	105.04	111.82
1	A	121	GLN	CA-CB-CG	-5.84	102.41	114.10
1	A	646	HIS	CB-CG-CD2	-5.83	123.62	131.20
1	A	115	ARG	NE-CZ-NH2	-5.83	113.95	119.20
1	A	539	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	A	360	ASN	OD1-CG-ND2	-5.79	116.81	122.60
1	A	583	LEU	N-CA-C	5.78	117.58	111.28
1	A	332	HIS	CB-CG-CD2	-5.78	123.69	131.20
1	A	368	ARG	CA-CB-CG	-5.78	102.54	114.10
1	A	402	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	46	HIS	CB-CG-ND1	5.77	131.35	122.70
1	A	626	HIS	CB-CG-CD2	-5.75	123.72	131.20
1	A	4	LYS	CA-CB-CG	-5.75	102.60	114.10
1	A	519	HIS	CA-CB-CG	-5.73	108.07	113.80
1	A	147	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	9	HIS	CB-CG-CD2	-5.71	123.77	131.20
1	A	327	THR	OG1-CB-CG2	5.71	120.71	109.30
1	A	574	GLY	CA-C-N	5.71	125.38	119.56
1	A	574	GLY	C-N-CA	5.71	125.38	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	ASP	N-CA-CB	-5.68	104.04	111.09
1	A	287	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	407	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	625	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	A	379	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	A	724	THR	CA-CB-OG1	-5.58	101.23	109.60
1	A	729	HIS	CB-CG-ND1	5.56	131.04	122.70
1	A	596	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	167	HIS	CB-CG-CD2	-5.54	123.99	131.20
1	A	260	GLY	N-CA-C	-5.53	108.58	114.67
1	A	641	GLY	CA-C-O	5.49	127.75	121.05
1	A	524	SER	N-CA-C	5.49	122.48	110.80
1	A	522	LYS	CA-C-O	5.48	125.97	119.56
1	A	165	ASP	O-C-N	-5.44	117.53	123.52
1	A	523	ASP	N-CA-C	-5.43	99.24	110.80
1	A	585	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	A	193	ILE	CA-C-N	5.41	125.42	119.90
1	A	193	ILE	C-N-CA	5.41	125.42	119.90
1	A	717	HIS	CA-C-N	5.40	125.04	119.05
1	A	717	HIS	C-N-CA	5.40	125.04	119.05
1	A	410	ARG	NE-CZ-NH1	5.37	126.86	121.50
1	A	674	LYS	N-CA-C	5.36	117.87	111.71
1	A	626	HIS	CA-CB-CG	-5.35	108.45	113.80
1	A	582	HIS	CB-CG-ND1	5.33	130.70	122.70
1	A	637	ASN	CB-CG-ND2	5.33	124.40	116.40
1	A	616	VAL	CA-C-N	5.33	124.78	119.24
1	A	616	VAL	C-N-CA	5.33	124.78	119.24
1	A	666	ARG	CG-CD-NE	-5.29	100.37	112.00
1	A	195	TRP	CG-CD1-NE1	-5.27	103.35	110.20
1	A	2	ARG	N-CA-C	-5.27	96.25	111.00
1	A	390	THR	CA-C-N	5.26	125.18	119.76
1	A	390	THR	C-N-CA	5.26	125.18	119.76
1	A	537	ARG	CA-CB-CG	-5.24	103.62	114.10
1	A	346	TRP	CE2-CD2-CG	-5.22	100.93	107.20
1	A	589	ASN	CB-CG-ND2	5.21	124.22	116.40
1	A	450	THR	N-CA-C	5.21	118.34	110.64
1	A	68	ARG	CA-CB-CG	5.20	124.50	114.10
1	A	665	ALA	N-CA-C	-5.20	103.54	110.55
1	A	306	HIS	CB-CG-CD2	-5.19	124.45	131.20
1	A	460	HIS	CB-CG-ND1	5.17	130.46	122.70
1	A	444	SER	N-CA-C	-5.17	105.22	112.25
1	A	236	ALA	N-CA-C	5.17	117.67	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	717	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	675	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	412	VAL	N-CA-CB	5.15	119.72	111.23
1	A	121	GLN	N-CA-C	5.14	117.55	111.33
1	A	357	SER	CA-CB-OG	5.14	121.37	111.10
1	A	618	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	536	GLN	N-CA-C	-5.12	107.09	113.38
1	A	522	LYS	CA-C-N	5.11	131.31	121.54
1	A	522	LYS	C-N-CA	5.11	131.31	121.54
1	A	379	HIS	CA-CB-CG	-5.07	108.73	113.80
1	A	580	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	A	168	THR	CA-C-N	5.05	126.16	119.84
1	A	168	THR	C-N-CA	5.05	126.16	119.84
1	A	399	THR	O-C-N	-5.04	116.40	122.15
1	A	63	ARG	CA-CB-CG	-5.01	104.07	114.10
1	A	360	ASN	CB-CG-ND2	5.01	123.92	116.40
1	A	374	LYS	CB-CG-CD	5.00	122.81	111.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide
1	A	580	ARG	Sidechain
1	A	666	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5812	0	5793	54	0
2	A	8	0	0	0	0
3	A	13	5	5	2	0
4	A	290	2	0	1	0
All	All	6123	7	5798	55	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HH22	1:A:439:ASN:HD21	1.24	0.84
1:A:13:HIS:HB3	4:A:1193:HOH:O	1.85	0.77
1:A:228:LEU:HD23	1:A:263:ILE:HD12	1.69	0.74
1:A:430:ARG:HH22	1:A:439:ASN:ND2	1.86	0.73
1:A:250:CYS:HA	1:A:253:MET:HE3	1.74	0.69
1:A:566:THR:HG22	1:A:568:ASP:H	1.59	0.67
1:A:384:LYS:HD3	1:A:476:GLY:HA3	1.77	0.66
1:A:546:LYS:HD3	1:A:741:ALA:O	1.96	0.65
3:A:755:NTC:O4	3:A:755:NTC:H22	1.91	0.61
1:A:49:ASP:OD2	1:A:52:ASN:HB2	2.01	0.59
1:A:165:ASP:OD1	3:A:755:NTC:H21	2.02	0.59
1:A:517:TYR:OH	1:A:519:HIS:HD2	1.87	0.58
1:A:752:GLN:O	1:A:754:LYS:HG3	2.04	0.57
1:A:402:ARG:HD2	1:A:403:ASP:OD1	2.05	0.57
1:A:277:LYS:HG3	1:A:289:ALA:HB1	1.87	0.56
1:A:336:GLU:O	1:A:340:VAL:HG23	2.05	0.56
1:A:754:LYS:HZ2	1:A:754:LYS:C	2.13	0.56
1:A:428:TRP:CZ2	1:A:430:ARG:HD3	2.43	0.54
1:A:17:ARG:NH2	1:A:20:LEU:HD23	2.22	0.54
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.73	0.53
1:A:430:ARG:NH2	1:A:439:ASN:HD21	2.01	0.52
1:A:430:ARG:HD2	1:A:432:ASP:OD1	2.09	0.52
1:A:622:TYR:O	1:A:626:HIS:HD2	1.93	0.52
1:A:552:LEU:HD23	1:A:629:ARG:HH21	1.75	0.51
1:A:517:TYR:OH	1:A:519:HIS:CD2	2.64	0.50
1:A:233:GLY:O	1:A:265:ALA:HA	2.11	0.49
1:A:110:GLU:O	1:A:114:ARG:HG3	2.13	0.49
1:A:2:ARG:HE	1:A:3:ALA:N	2.11	0.48
1:A:277:LYS:NZ	1:A:293:ASP:OD2	2.47	0.48
1:A:145:ILE:HG21	1:A:358:CYS:HB3	1.96	0.47
1:A:517:TYR:CE2	1:A:519:HIS:HD2	2.33	0.47
1:A:341:ALA:HA	1:A:346:TRP:CE3	2.50	0.47
1:A:208:THR:O	1:A:315:LEU:HB2	2.15	0.47
1:A:230:VAL:HA	1:A:263:ILE:HA	1.98	0.46
1:A:278:LYS:NZ	1:A:504:GLU:OE2	2.50	0.44
1:A:374:LYS:HD2	1:A:375:GLN:HG3	1.98	0.44
1:A:652:ARG:HD3	1:A:677:LEU:HG	1.98	0.44
1:A:143:SER:HB3	1:A:516:THR:HB	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:SER:HA	1:A:464:THR:O	2.18	0.44
1:A:589:ASN:C	1:A:589:ASN:HD22	2.26	0.44
1:A:717:HIS:HD2	1:A:721:THR:HB	1.83	0.44
1:A:754:LYS:C	1:A:754:LYS:NZ	2.75	0.44
1:A:438:LYS:HZ2	1:A:458:GLU:CD	2.25	0.43
1:A:456:ASN:HA	1:A:457:PRO:HD2	1.87	0.43
1:A:121:GLN:O	1:A:125:ASN:HB2	2.18	0.42
1:A:576:TRP:CE2	1:A:589:ASN:HB3	2.54	0.42
1:A:675:GLN:NE2	1:A:675:GLN:HA	2.34	0.42
1:A:325:PRO:HG2	1:A:326:PHE:CD1	2.55	0.41
1:A:90:LYS:HD2	1:A:134:TYR:O	2.20	0.41
1:A:451:GLY:O	1:A:455:ALA:HA	2.20	0.41
1:A:330:LEU:HD22	1:A:332:HIS:CE1	2.55	0.41
1:A:228:LEU:O	1:A:232:GLY:HA3	2.21	0.41
1:A:69:VAL:O	1:A:95:SER:HA	2.21	0.40
1:A:169:PRO:O	1:A:257:CYS:HB3	2.22	0.40
1:A:522:LYS:CE	1:A:522:LYS:HA	2.52	0.40

There are no symmetry-related clashes.

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	751/754 (100%)	716 (95%)	31 (4%)	4 (0%)	24 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	SER
1	A	525	SER
1	A	109	GLY
1	A	753	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	621/622 (100%)	576 (93%)	45 (7%)	13 7

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	20	LEU
1	A	107	LEU
1	A	110	GLU
1	A	121	GLN
1	A	125	ASN
1	A	174	LEU
1	A	208	THR
1	A	228	LEU
1	A	247	SER
1	A	310	LEU
1	A	315	LEU
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	327	THR
1	A	330	LEU
1	A	344	GLU
1	A	374	LYS
1	A	382	LYS
1	A	384	LYS
1	A	412	VAL
1	A	425	ILE
1	A	430	ARG
1	A	433	ILE
1	A	435	LYS
1	A	442	VAL
1	A	487	LEU
1	A	490	LYS
1	A	496	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	497	LEU
1	A	498	GLU
1	A	514	GLN
1	A	522	LYS
1	A	550	LYS
1	A	553	GLU
1	A	562	LYS
1	A	578	LYS
1	A	589	ASN
1	A	631	VAL
1	A	657	ARG
1	A	702	LEU
1	A	704	ASP
1	A	747	ARG
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	77	GLN
1	A	106	GLN
1	A	125	ASN
1	A	148	GLN
1	A	321	HIS
1	A	395	GLN
1	A	419	ASN
1	A	439	ASN
1	A	453	ASN
1	A	514	GLN
1	A	519	HIS
1	A	536	GLN
1	A	585	ASN
1	A	589	ASN
1	A	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	A	999	4,1	0,12,12	-	-	-		
3	NTC	A	755	-	9,12,12	2.19	3 (33%)	14,17,17	3.29	4 (28%)

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	SF4	A	999	4,1	-	-	0/6/5/5
3	NTC	A	755	-	-	8/15/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	755	NTC	C3-C6	3.80	1.57	1.53
3	A	755	NTC	C4-C3	3.80	1.58	1.54
3	A	755	NTC	O4-C5	-2.93	1.21	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	755	NTC	C2-C3-C4	-8.25	92.31	109.08
3	A	755	NTC	O7-C3-C4	6.19	123.50	109.38
3	A	755	NTC	C3-C4-C5	4.31	125.72	113.92
3	A	755	NTC	O6-C6-C3	2.88	118.67	113.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	755	NTC	N1-C2-C3-C4
3	A	755	NTC	N1-C2-C3-C6
3	A	755	NTC	C4-C3-C6-O5
3	A	755	NTC	C4-C3-C6-O6
3	A	755	NTC	C2-C3-C4-C5
3	A	755	NTC	C6-C3-C4-C5
3	A	755	NTC	N1-C2-C3-O7
3	A	755	NTC	C2-C3-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	755	NTC	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.