



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:30 PM UTC

PDB ID : 6ACN / pdb_00006acn
Title : STRUCTURE OF ACTIVATED ACONITASE. FORMATION OF THE
(4FE-4S) CLUSTER IN THE CRYSTAL
Authors : Robbins, A.H.; Stout, C.D.
Deposited on : 1990-01-16
Resolution : 2.50 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

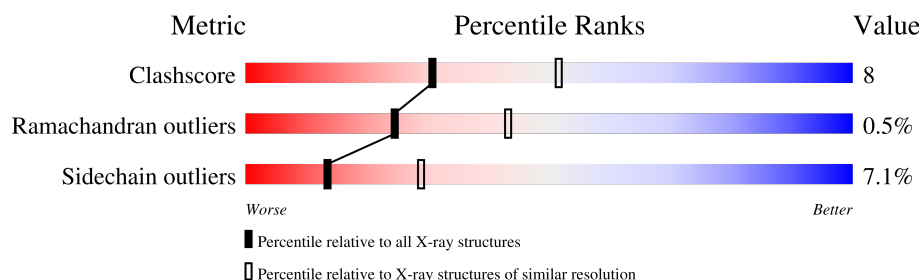
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	 60% 32% 7%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6255 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ACONITASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	754	5823	3671	1035	1095	22	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	647	SER	ARG	conflict	UNP P16276

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



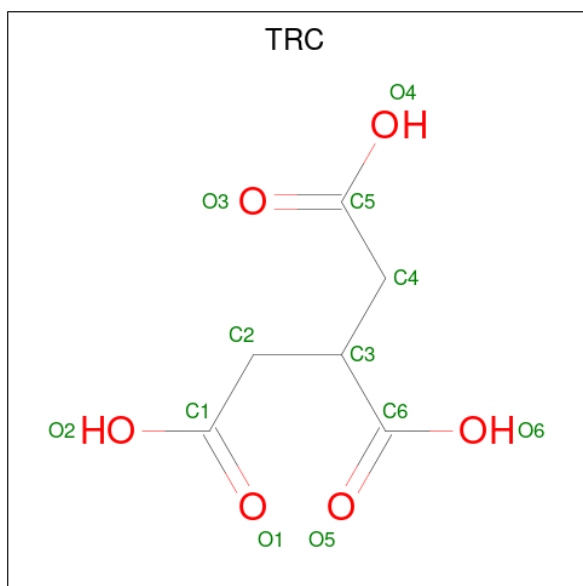
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 4 is TRICARBALLYLIC ACID (CCD ID: TRC) (formula: $C_6H_8O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is water.

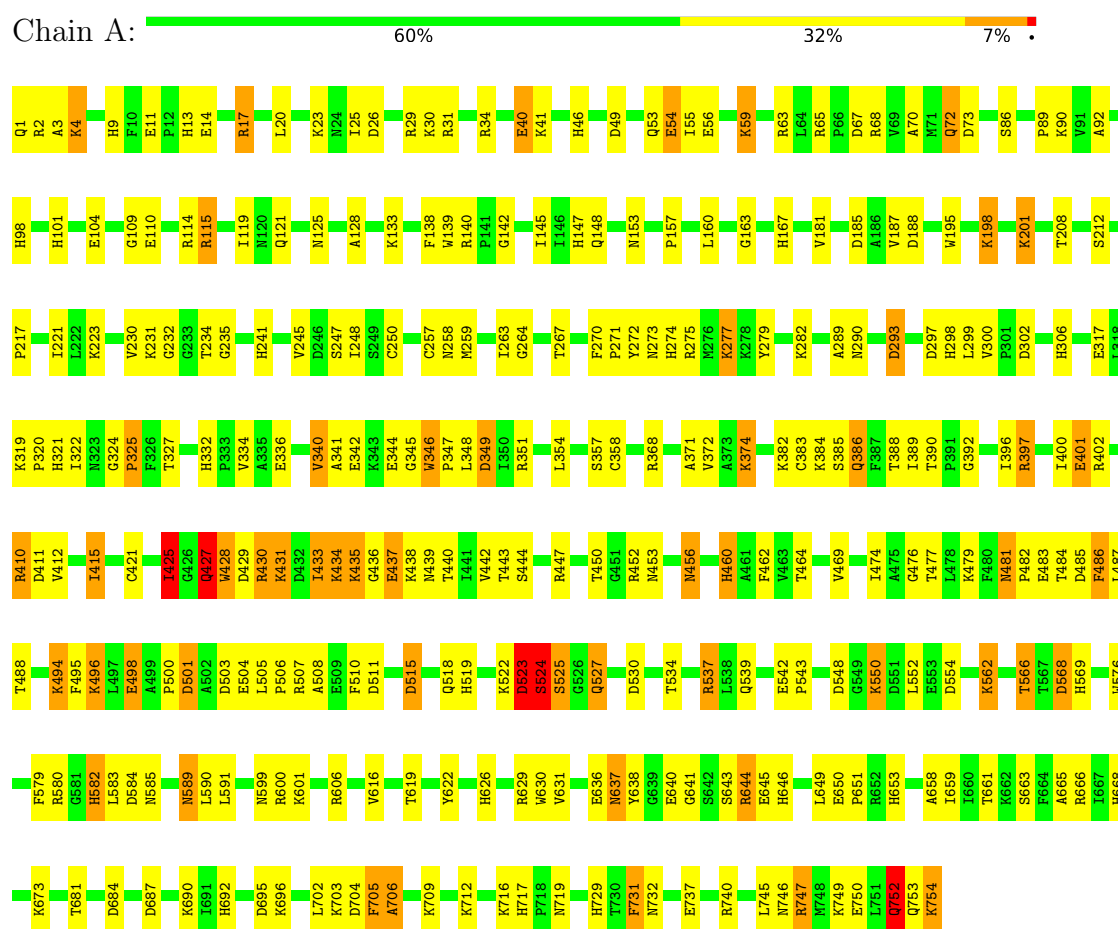
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	407	Total 407	O 407	0	0

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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.60Å 72.00Å 72.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6255	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, TRC, SO4, PCA

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	1.23	35/5943 (0.6%)	2.08	234/8053 (2.9%)

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	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	THR	CA-CB	10.58	1.66	1.53
1	A	98	HIS	CD2-NE2	-7.54	1.29	1.37
1	A	9	HIS	CD2-NE2	-7.50	1.29	1.37
1	A	167	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	646	HIS	CD2-NE2	-7.16	1.29	1.37
1	A	460	HIS	CD2-NE2	-7.05	1.30	1.37
1	A	653	HIS	CD2-NE2	-7.01	1.30	1.37
1	A	306	HIS	CD2-NE2	-6.94	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.85	1.30	1.37
1	A	298	HIS	CD2-NE2	-6.81	1.30	1.37
1	A	46	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	332	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	582	HIS	CD2-NE2	-6.54	1.30	1.37
1	A	321	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	241	HIS	CD2-NE2	-6.34	1.30	1.37
1	A	4	LYS	CA-CB	-6.29	1.47	1.53
1	A	668	HIS	CD2-NE2	-6.28	1.30	1.37
1	A	729	HIS	CD2-NE2	-6.10	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	HIS	CD2-NE2	-6.05	1.31	1.37
1	A	98	HIS	CG-ND1	-6.00	1.31	1.38
1	A	13	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	626	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	692	HIS	CD2-NE2	-5.98	1.31	1.37
1	A	101	HIS	CD2-NE2	-5.90	1.31	1.37
1	A	114	ARG	NE-CZ	5.83	1.39	1.33
1	A	9	HIS	CG-ND1	-5.65	1.32	1.38
1	A	519	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	464	THR	CA-CB	5.57	1.59	1.54
1	A	321	HIS	CG-ND1	-5.57	1.32	1.38
1	A	13	HIS	CB-CG	5.38	1.57	1.50
1	A	569	HIS	CD2-NE2	-5.37	1.31	1.37
1	A	63	ARG	NE-CZ	5.23	1.38	1.33
1	A	147	HIS	CG-ND1	-5.17	1.32	1.38
1	A	101	HIS	CG-ND1	-5.11	1.32	1.38
1	A	274	HIS	CD2-NE2	-5.02	1.32	1.37

All (234) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	548	ASP	CA-CB-CG	12.08	124.68	112.60
1	A	447	ARG	NE-CZ-NH2	10.40	128.56	119.20
1	A	582	HIS	CB-CG-CD2	-9.57	118.76	131.20
1	A	705	PHE	CA-CB-CG	9.24	123.04	113.80
1	A	125	ASN	CA-CB-CG	-9.21	103.39	112.60
1	A	589	ASN	CA-CB-CG	9.19	121.79	112.60
1	A	507	ARG	N-CA-C	-8.90	101.55	111.07
1	A	447	ARG	NE-CZ-NH1	-8.73	112.77	121.50
1	A	582	HIS	CB-CG-ND1	8.59	135.58	122.70
1	A	72	GLN	N-CA-CB	-8.48	96.07	110.83
1	A	188	ASP	CA-CB-CG	8.27	120.87	112.60
1	A	410	ARG	NE-CZ-NH1	-8.25	113.25	121.50
1	A	485	ASP	N-CA-C	8.22	121.20	110.43
1	A	523	ASP	CA-CB-CG	8.15	120.75	112.60
1	A	486	PHE	CA-CB-CG	-8.10	105.70	113.80
1	A	510	PHE	CA-CB-CG	7.95	121.75	113.80
1	A	410	ARG	NE-CZ-NH2	7.84	126.26	119.20
1	A	274	HIS	CB-CG-CD2	-7.80	121.06	131.20
1	A	518	GLN	OE1-CD-NE2	-7.71	114.89	122.60
1	A	746	ASN	CA-CB-CG	7.70	120.30	112.60
1	A	498	GLU	CA-CB-CG	7.69	129.48	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	THR	N-CA-CB	-7.52	97.66	111.13
1	A	101	HIS	CB-CG-ND1	7.41	133.81	122.70
1	A	500	PRO	CA-C-O	7.35	130.09	121.56
1	A	584	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	72	GLN	CA-CB-CG	7.31	128.72	114.10
1	A	374	LYS	CB-CG-CD	7.21	127.89	111.30
1	A	641	GLY	N-CA-C	7.04	118.54	111.21
1	A	464	THR	O-C-N	-7.03	117.83	123.11
1	A	101	HIS	CB-CG-CD2	-7.02	122.07	131.20
1	A	719	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	A	585	ASN	CB-CG-ND2	6.98	126.87	116.40
1	A	460	HIS	CB-CG-CD2	-6.97	122.14	131.20
1	A	382	LYS	N-CA-CB	-6.94	99.62	111.21
1	A	332	HIS	CB-CG-CD2	-6.92	122.21	131.20
1	A	599	ASN	OD1-CG-ND2	-6.91	115.69	122.60
1	A	121	GLN	CB-CG-CD	6.88	124.30	112.60
1	A	46	HIS	CB-CG-CD2	-6.88	122.26	131.20
1	A	73	ASP	CA-CB-CG	6.85	119.45	112.60
1	A	450	THR	N-CA-C	6.82	119.68	109.25
1	A	643	SER	N-CA-C	6.81	120.85	112.54
1	A	250	CYS	O-C-N	-6.80	114.91	122.12
1	A	729	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	A	646	HIS	CB-CG-CD2	-6.75	122.43	131.20
1	A	72	GLN	CB-CA-C	6.73	122.22	109.37
1	A	637	ASN	CB-CG-ND2	6.72	126.48	116.40
1	A	644	ARG	CA-CB-CG	6.72	127.55	114.10
1	A	589	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	A	524	SER	N-CA-C	6.67	125.01	110.80
1	A	348	LEU	N-CA-C	6.67	120.63	112.23
1	A	566	THR	N-CA-CB	-6.67	99.80	110.46
1	A	167	HIS	CB-CG-CD2	-6.65	122.56	131.20
1	A	494	LYS	CG-CD-CE	-6.63	96.04	111.30
1	A	167	HIS	CB-CG-ND1	6.56	132.54	122.70
1	A	585	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	A	195	TRP	CG-CD1-NE1	-6.54	101.70	110.20
1	A	503	ASP	CA-CB-CG	6.50	119.10	112.60
1	A	195	TRP	CG-CD2-CE3	6.49	140.39	133.90
1	A	267	THR	CA-CB-OG1	-6.47	99.89	109.60
1	A	300	VAL	O-C-N	-6.47	117.19	121.72
1	A	705	PHE	N-CA-C	-6.46	100.10	109.59
1	A	298	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	637	ASN	OD1-CG-ND2	-6.45	116.15	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	THR	CA-CB-OG1	-6.45	99.93	109.60
1	A	63	ARG	N-CA-CB	-6.43	99.80	110.47
1	A	92	ALA	N-CA-C	6.36	121.20	113.38
1	A	402	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	115	ARG	NE-CZ-NH2	6.36	124.92	119.20
1	A	241	HIS	CB-CG-CD2	-6.36	122.94	131.20
1	A	59	LYS	O-C-N	-6.33	114.17	122.59
1	A	732	ASN	OD1-CG-ND2	-6.33	116.27	122.60
1	A	86	SER	N-CA-C	-6.31	104.50	111.82
1	A	282	LYS	CB-CG-CD	6.30	125.79	111.30
1	A	425	ILE	CB-CA-C	-6.30	100.79	111.37
1	A	340	VAL	CB-CA-C	-6.25	103.83	112.02
1	A	55	ILE	N-CA-C	6.24	116.60	107.37
1	A	250	CYS	N-CA-CB	-6.23	100.96	110.12
1	A	293	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	524	SER	CA-C-O	6.20	129.38	120.51
1	A	534	THR	N-CA-CB	-6.20	101.47	110.70
1	A	569	HIS	ND1-CG-CD2	6.17	112.28	106.10
1	A	274	HIS	CB-CG-ND1	6.13	131.89	122.70
1	A	17	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	372	VAL	N-CA-C	-6.09	105.78	111.45
1	A	245	VAL	N-CA-CB	-6.08	103.76	110.51
1	A	140	ARG	N-CA-CB	-6.08	100.44	109.98
1	A	298	HIS	CB-CG-CD2	-6.06	123.33	131.20
1	A	147	HIS	CA-CB-CG	-6.05	107.75	113.80
1	A	591	LEU	N-CA-C	6.04	119.87	111.90
1	A	160	LEU	N-CA-C	-6.02	97.49	108.02
1	A	666	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	153	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	637	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	437	GLU	CA-C-O	-5.90	114.66	121.15
1	A	13	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	A	433	ILE	O-C-N	5.88	129.20	123.03
1	A	14	GLU	N-CA-C	-5.86	98.86	108.41
1	A	616	VAL	CA-C-N	5.85	125.54	119.05
1	A	616	VAL	C-N-CA	5.85	125.54	119.05
1	A	644	ARG	N-CA-CB	-5.85	100.60	110.49
1	A	460	HIS	CB-CG-ND1	5.85	131.47	122.70
1	A	481	ASN	CA-C-N	5.84	125.53	119.05
1	A	481	ASN	C-N-CA	5.84	125.53	119.05
1	A	297	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	579	PHE	CA-CB-CG	5.82	119.62	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	PRO	CA-C-N	-5.81	112.84	122.08
1	A	325	PRO	C-N-CA	-5.81	112.84	122.08
1	A	397	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	A	519	HIS	CB-CG-CD2	-5.80	123.66	131.20
1	A	427	GLN	N-CA-CB	-5.78	102.77	110.57
1	A	340	VAL	N-CA-CB	5.77	117.96	110.57
1	A	153	ASN	OD1-CG-ND2	-5.76	116.84	122.60
1	A	195	TRP	CB-CG-CD1	-5.76	118.27	126.90
1	A	342	GLU	O-C-N	-5.75	115.88	122.09
1	A	346	TRP	CG-CD2-CE3	5.73	139.63	133.90
1	A	515	ASP	N-CA-CB	-5.72	103.09	112.25
1	A	436	GLY	N-CA-C	-5.72	107.78	115.21
1	A	447	ARG	N-CA-CB	-5.70	100.76	110.16
1	A	518	GLN	CG-CD-NE2	5.69	124.94	116.40
1	A	684	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	273	ASN	CA-CB-CG	5.68	118.28	112.60
1	A	212	SER	N-CA-C	5.66	118.42	108.75
1	A	712	LYS	N-CA-CB	-5.64	101.71	110.57
1	A	402	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A	17	ARG	N-CA-C	5.62	117.10	109.11
1	A	3	ALA	O-C-N	-5.62	116.39	122.79
1	A	488	THR	CA-C-N	5.61	126.87	120.53
1	A	488	THR	C-N-CA	5.61	126.87	120.53
1	A	438	LYS	CB-CG-CD	5.61	124.19	111.30
1	A	195	TRP	CE2-CD2-CG	-5.60	100.48	107.20
1	A	695	ASP	CA-CB-CG	5.58	118.19	112.60
1	A	589	ASN	CB-CG-ND2	5.58	124.77	116.40
1	A	752	GLN	CG-CD-NE2	5.58	124.77	116.40
1	A	434	LYS	O-C-N	-5.57	116.67	122.96
1	A	167	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	495	PHE	N-CA-C	-5.56	100.28	108.79
1	A	712	LYS	CA-CB-CG	5.55	125.21	114.10
1	A	133	LYS	N-CA-C	5.55	117.14	111.14
1	A	511	ASP	O-C-N	-5.55	116.59	121.31
1	A	345	GLY	CA-C-O	5.53	124.84	118.98
1	A	241	HIS	O-C-N	-5.52	117.46	123.26
1	A	712	LYS	CB-CA-C	5.49	119.22	109.72
1	A	717	HIS	CB-CG-CD2	-5.49	124.06	131.20
1	A	537	ARG	N-CA-CB	-5.49	102.68	110.81
1	A	447	ARG	CB-CA-C	5.49	118.80	109.80
1	A	65	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	A	453	ASN	OD1-CG-ND2	-5.46	117.14	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	390	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	580	ARG	CB-CG-CD	5.45	123.83	111.30
1	A	63	ARG	CA-CB-CG	5.44	124.98	114.10
1	A	195	TRP	CD1-CG-CD2	5.44	115.01	106.30
1	A	525	SER	N-CA-C	-5.43	99.06	108.52
1	A	477	THR	O-C-N	5.43	129.46	123.33
1	A	54	GLU	CA-CB-CG	5.41	124.93	114.10
1	A	566	THR	O-C-N	-5.40	116.89	122.94
1	A	31	ARG	N-CA-C	-5.40	104.94	112.45
1	A	629	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	68	ARG	CA-CB-CG	5.38	124.86	114.10
1	A	270	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	653	HIS	CB-CG-CD2	-5.37	124.22	131.20
1	A	447	ARG	CA-CB-CG	5.37	124.83	114.10
1	A	53	GLN	OE1-CD-NE2	-5.36	117.24	122.60
1	A	332	HIS	O-C-N	-5.36	116.31	121.94
1	A	336	GLU	N-CA-C	5.36	119.82	113.28
1	A	14	GLU	N-CA-CB	-5.35	102.30	110.65
1	A	54	GLU	CB-CG-CD	5.34	121.69	112.60
1	A	507	ARG	N-CA-CB	-5.34	102.26	110.01
1	A	630	TRP	CG-CD2-CE3	5.34	139.24	133.90
1	A	290	ASN	OD1-CG-ND2	-5.34	117.26	122.60
1	A	606	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	382	LYS	CA-CB-CG	5.33	124.77	114.10
1	A	290	ASN	CA-CB-CG	5.33	117.93	112.60
1	A	11	GLU	CA-C-N	5.33	125.41	119.87
1	A	11	GLU	C-N-CA	5.33	125.41	119.87
1	A	665	ALA	N-CA-C	-5.30	101.89	110.32
1	A	258	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	498	GLU	N-CA-C	-5.27	102.47	110.28
1	A	267	THR	CA-CB-CG2	5.26	119.44	110.50
1	A	140	ARG	CB-CA-C	5.26	117.83	109.52
1	A	148	GLN	CA-CB-CG	-5.26	103.58	114.10
1	A	386	GLN	N-CA-C	-5.26	102.50	110.28
1	A	601	LYS	CA-CB-CG	5.25	124.59	114.10
1	A	636	GLU	N-CA-C	5.25	118.78	109.96
1	A	208	THR	CB-CA-C	5.25	120.03	109.38
1	A	706	ALA	CA-C-N	5.25	125.25	119.90
1	A	706	ALA	C-N-CA	5.25	125.25	119.90
1	A	554	ASP	N-CA-C	5.24	118.62	111.39
1	A	527	GLN	N-CA-C	-5.24	100.77	109.46
1	A	9	HIS	CB-CG-CD2	-5.22	124.41	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110	GLU	CB-CG-CD	5.22	121.47	112.60
1	A	142	GLY	N-CA-C	-5.22	108.14	114.92
1	A	232	GLY	N-CA-C	5.22	118.95	112.64
1	A	49	ASP	CA-C-N	5.22	125.02	119.28
1	A	49	ASP	C-N-CA	5.22	125.02	119.28
1	A	357	SER	CA-CB-OG	5.21	121.53	111.10
1	A	89	PRO	N-CA-C	5.18	120.34	113.40
1	A	629	ARG	CB-CG-CD	-5.17	99.40	111.30
1	A	258	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	53	GLN	CG-CD-NE2	5.16	124.15	116.40
1	A	201	LYS	N-CA-C	-5.16	103.10	110.59
1	A	271	PRO	CA-C-O	-5.16	115.56	121.86
1	A	299	LEU	N-CA-C	5.16	118.89	112.59
1	A	277	LYS	CA-C-N	5.16	127.15	120.44
1	A	277	LYS	C-N-CA	5.16	127.15	120.44
1	A	576	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	444	SER	CA-CB-OG	5.15	121.41	111.10
1	A	530	ASP	CB-CA-C	-5.15	101.90	110.14
1	A	257	CYS	CA-C-N	5.15	127.49	120.54
1	A	257	CYS	C-N-CA	5.15	127.49	120.54
1	A	98	HIS	CB-CG-CD2	-5.14	124.52	131.20
1	A	663	SER	O-C-N	-5.14	117.72	123.48
1	A	40	GLU	N-CA-C	-5.14	105.59	111.14
1	A	427	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	746	ASN	N-CA-C	-5.13	105.68	111.28
1	A	121	GLN	OE1-CD-NE2	-5.11	117.49	122.60
1	A	139	TRP	CA-C-O	5.11	125.83	120.36
1	A	731	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	501	ASP	O-C-N	-5.11	117.23	123.30
1	A	104	GLU	N-CA-C	5.08	117.90	109.46
1	A	583	LEU	CA-C-O	-5.08	115.48	120.82
1	A	554	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	401	GLU	N-CA-C	-5.05	105.42	111.03
1	A	729	HIS	CB-CG-ND1	5.05	130.27	122.70
1	A	342	GLU	CA-C-O	-5.05	115.50	120.70
1	A	17	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	A	346	TRP	CE2-CD2-CG	-5.03	101.16	107.20
1	A	411	ASP	O-C-N	-5.02	116.80	122.12
1	A	368	ARG	N-CA-C	-5.02	105.89	111.36
1	A	67	ASP	N-CA-C	5.01	117.86	111.69
1	A	302	ASP	CA-C-N	5.01	125.29	119.93
1	A	302	ASP	C-N-CA	5.01	125.29	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	TRP	CG-CD2-CE3	5.01	138.91	133.90
1	A	456	ASN	N-CA-C	-5.01	98.78	108.59
1	A	606	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5823	0	5811	96	0
2	A	5	0	0	0	0
3	A	8	0	0	1	0
4	A	12	0	5	1	0
5	A	407	0	0	10	0
All	All	6255	0	5816	97	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 8.

All (97) 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:384:LYS:HD2	1:A:476:GLY:HA3	1.57	0.85
1:A:371:ALA:HA	1:A:374:LYS:HD3	1.59	0.83
1:A:434:LYS:HB3	1:A:437:GLU:HG3	1.59	0.83
1:A:750:GLU:HA	1:A:754:LYS:HA	1.64	0.80
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.66	0.77
1:A:277:LYS:HG2	1:A:289:ALA:HB1	1.69	0.73
3:A:999:SF4:FE4	5:A:806:HOH:O	1.44	0.70
1:A:198:LYS:HE2	5:A:823:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:GLU:HG2	5:A:970:HOH:O	1.95	0.66
1:A:384:LYS:HB2	1:A:474:ILE:O	1.98	0.64
1:A:752:GLN:HB2	1:A:753:GLN:HG2	1.80	0.64
1:A:354:LEU:HD13	1:A:443:THR:HG22	1.79	0.63
1:A:661:THR:O	1:A:681:THR:HA	2.00	0.61
1:A:145:ILE:HD12	1:A:392:GLY:HA2	1.84	0.58
1:A:54:GLU:HB2	5:A:1008:HOH:O	2.03	0.58
1:A:29:ARG:HH21	1:A:29:ARG:HG3	1.68	0.58
1:A:637:ASN:O	1:A:640:GLU:HB2	2.04	0.58
1:A:279:TYR:HD2	1:A:505:LEU:HD21	1.70	0.57
1:A:498:GLU:HB2	5:A:1118:HOH:O	2.03	0.56
1:A:428:TRP:CH2	1:A:430:ARG:HD3	2.42	0.55
1:A:745:LEU:O	1:A:749:LYS:HG3	2.07	0.55
1:A:631:VAL:HG22	1:A:658:ALA:HB3	1.88	0.55
1:A:496:LYS:NZ	1:A:496:LYS:HB2	2.22	0.54
1:A:341:ALA:HA	1:A:346:TRP:HB2	1.89	0.54
1:A:322:ILE:HG12	1:A:462:PHE:HB3	1.89	0.54
1:A:56:GLU:HB3	1:A:59:LYS:HB2	1.90	0.53
1:A:550:LYS:HA	1:A:703:LYS:HZ1	1.74	0.53
1:A:115:ARG:O	1:A:119:ILE:HG12	2.10	0.52
1:A:539:GLN:HB2	1:A:582:HIS:CD2	2.45	0.52
1:A:550:LYS:HA	1:A:703:LYS:NZ	2.24	0.52
1:A:487:LEU:O	1:A:494:LYS:HA	2.09	0.51
1:A:221:ILE:CG1	1:A:259:MET:HB3	2.39	0.51
1:A:524:SER:HB3	1:A:527:GLN:HB2	1.93	0.51
1:A:566:THR:HG22	1:A:568:ASP:H	1.75	0.51
1:A:70:ALA:O	1:A:163:GLY:HA2	2.13	0.49
1:A:322:ILE:CG1	1:A:462:PHE:HB3	2.42	0.49
1:A:706:ALA:HB3	1:A:709:LYS:HB2	1.95	0.49
1:A:347:PRO:HD2	1:A:460:HIS:CD2	2.48	0.48
1:A:430:ARG:HH12	1:A:439:ASN:HD21	1.61	0.48
1:A:371:ALA:CA	1:A:374:LYS:HD3	2.39	0.48
1:A:737:GLU:HB3	1:A:747:ARG:HD2	1.94	0.48
1:A:54:GLU:H	1:A:54:GLU:CD	2.22	0.48
1:A:479:LYS:HD2	1:A:479:LYS:HA	1.60	0.48
1:A:427:GLN:HE21	1:A:427:GLN:HA	1.79	0.47
1:A:320:PRO:HB2	1:A:334:VAL:CG2	2.45	0.47
1:A:230:VAL:HA	1:A:263:ILE:HA	1.97	0.46
1:A:388:THR:HG22	1:A:415:ILE:HG23	1.97	0.46
1:A:481:ASN:HA	1:A:482:PRO:HD3	1.83	0.46
1:A:25:ILE:O	1:A:29:ARG:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASP:OD2	1:A:384:LYS:NZ	2.49	0.45
1:A:645:GLU:HG3	1:A:649:LEU:HD12	1.98	0.45
1:A:401:GLU:CD	1:A:410:ARG:HH12	2.24	0.45
1:A:562:LYS:NZ	5:A:941:HOH:O	2.48	0.45
1:A:590:LEU:HD11	1:A:651:PRO:HG3	1.97	0.45
1:A:749:LYS:HB3	1:A:749:LYS:HE3	1.85	0.44
1:A:34:ARG:HH22	1:A:40:GLU:CD	2.25	0.44
1:A:217:PRO:HG3	1:A:248:ILE:HG23	1.98	0.44
1:A:673:LYS:HG2	1:A:731:PHE:CZ	2.52	0.44
1:A:41:LYS:NZ	5:A:1067:HOH:O	2.51	0.43
1:A:235:GLY:HA2	4:A:899:TRC:O3	2.17	0.43
1:A:351:ARG:NH1	1:A:433:ILE:HG22	2.33	0.43
1:A:562:LYS:O	1:A:562:LYS:HE2	2.18	0.43
1:A:619:THR:O	1:A:622:TYR:HB3	2.17	0.43
1:A:181:VAL:HB	1:A:185:ASP:HB2	2.00	0.43
1:A:435:LYS:HE2	1:A:456:ASN:HB2	2.00	0.43
1:A:231:LYS:NZ	5:A:1159:HOH:O	2.48	0.43
1:A:650:GLU:HB2	1:A:651:PRO:HD3	2.00	0.43
1:A:340:VAL:O	1:A:344:GLU:HB2	2.19	0.43
1:A:354:LEU:O	1:A:443:THR:HA	2.19	0.43
1:A:638:TYR:CE2	1:A:659:ILE:HG21	2.54	0.43
1:A:687:ASP:HA	1:A:690:LYS:HD3	2.00	0.42
1:A:157:PRO:HG2	1:A:272:TYR:CD1	2.54	0.42
1:A:397:ARG:NH1	5:A:1130:HOH:O	2.51	0.42
1:A:486:PHE:HB3	1:A:494:LYS:HB3	2.01	0.42
1:A:552:LEU:HG	1:A:702:LEU:HD11	2.01	0.42
1:A:506:PRO:HB2	1:A:508:ALA:O	2.19	0.42
1:A:234:THR:HA	1:A:264:GLY:O	2.20	0.42
1:A:659:ILE:HG22	1:A:661:THR:HG23	2.02	0.42
1:A:26:ASP:OD1	1:A:30:LYS:NZ	2.53	0.42
1:A:145:ILE:HG21	1:A:358:CYS:HB3	2.01	0.42
1:A:320:PRO:HB2	1:A:334:VAL:HG22	2.02	0.41
1:A:275:ARG:HH11	1:A:504:GLU:CD	2.27	0.41
1:A:452:ARG:NH2	5:A:995:HOH:O	2.54	0.41
1:A:277:LYS:NZ	1:A:293:ASP:OD1	2.49	0.41
1:A:442:VAL:HG12	1:A:469:VAL:HG22	2.03	0.41
1:A:383:CYS:HB3	1:A:385:SER:O	2.20	0.41
1:A:440:THR:HA	1:A:460:HIS:O	2.21	0.41
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.91	0.41
1:A:702:LEU:O	1:A:705:PHE:HB2	2.21	0.41
1:A:29:ARG:HH21	1:A:29:ARG:CG	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:O	1:A:400:ILE:HG12	2.20	0.41
1:A:429:ASP:OD1	1:A:431:LYS:NZ	2.54	0.41
1:A:29:ARG:HG3	1:A:29:ARG:NH2	2.36	0.40
1:A:128:ALA:HB2	1:A:138:PHE:CE2	2.57	0.40
1:A:696:LYS:HA	1:A:696:LYS:HD3	1.89	0.40
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.04	0.40
1:A:1:PCA:HG3	1:A:17:ARG:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	752/754 (100%)	709 (94%)	39 (5%)	4 (0%)	24 43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	A	524	SER
1	A	109	GLY
1	A	644	ARG

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/622 (100%)	578 (93%)	44 (7%)	13	29

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	LYS
1	A	20	LEU
1	A	23	LYS
1	A	72	GLN
1	A	90	LYS
1	A	187	VAL
1	A	198	LYS
1	A	201	LYS
1	A	223	LYS
1	A	247	SER
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	327	THR
1	A	349	ASP
1	A	386	GLN
1	A	389	ILE
1	A	412	VAL
1	A	415	ILE
1	A	425	ILE
1	A	427	GLN
1	A	430	ARG
1	A	431	LYS
1	A	435	LYS
1	A	483	GLU
1	A	496	LYS
1	A	501	ASP
1	A	515	ASP
1	A	522	LYS
1	A	523	ASP
1	A	525	SER
1	A	537	ARG
1	A	550	LYS
1	A	562	LYS
1	A	568	ASP
1	A	589	ASN
1	A	600	ARG

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Mol	Chain	Res	Type
1	A	704	ASP
1	A	716	LYS
1	A	740	ARG
1	A	747	ARG
1	A	752	GLN
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	33	ASN
1	A	77	GLN
1	A	106	GLN
1	A	427	GLN
1	A	456	ASN
1	A	539	GLN
1	A	671	ASN
1	A	675	GLN
1	A	722	GLN
1	A	753	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	0.98	0	9,10,12	0.83	0

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	SF4	A	999	1	0,12,12	-	-	-		
2	SO4	A	998	-	4,4,4	0.71	0	6,6,6	0.54	0
4	TRC	A	899	-	11,11,11	1.93	2 (18%)	14,14,14	1.13	1 (7%)

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
3	SF4	A	999	1	-	-	0/6/5/5
4	TRC	A	899	-	-	2/12/12/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	899	TRC	C3-C6	3.92	1.58	1.51
4	A	899	TRC	C2-C3	2.42	1.58	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	899	TRC	O4-C5-C4	2.49	121.74	114.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	899	TRC	C3-C4-C5-O3
4	A	899	TRC	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	SF4	1	0
4	A	899	TRC	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.