



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:58 AM UTC

PDB ID : 5ACN / pdb_00005acn
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 : 2.10 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

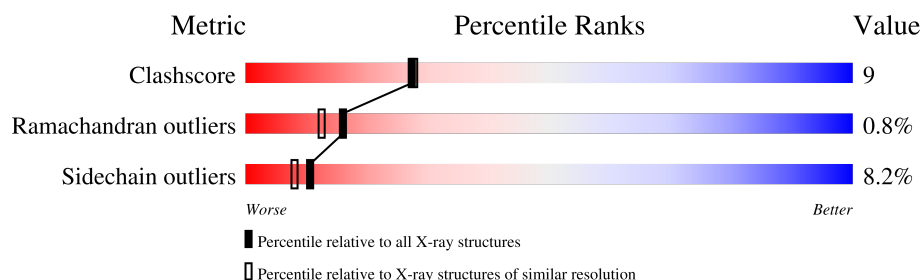
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 6254 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.

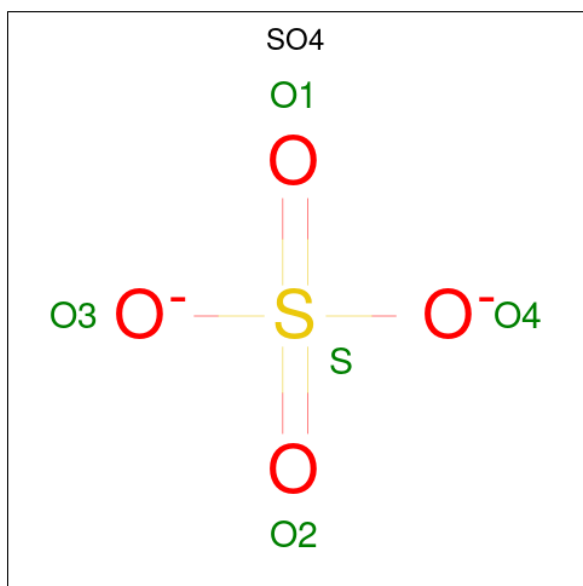
- Molecule 1 is a protein called ACONITASE.

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:

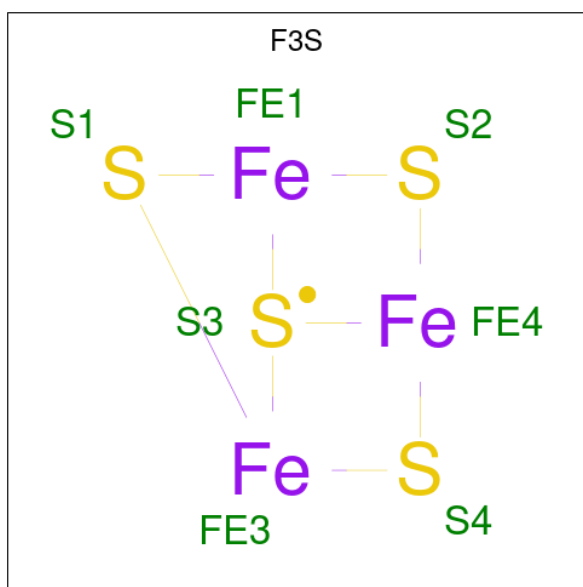
Chain	Residue	Modelled	Actual	Comment	Reference
A	647	SER	ARG	conflict	UNP P16276

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



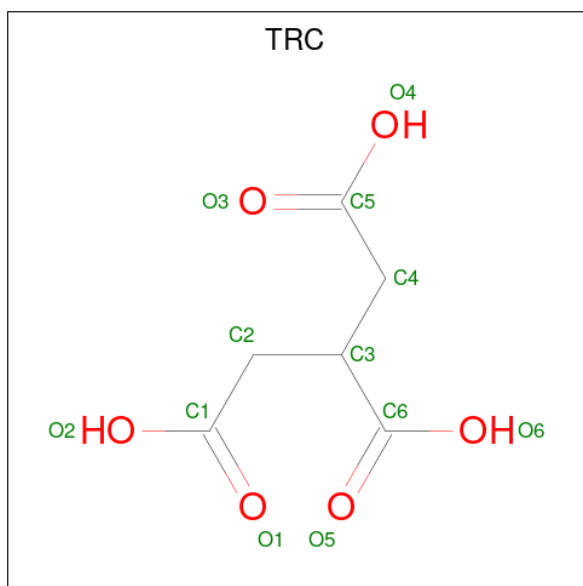
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	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.

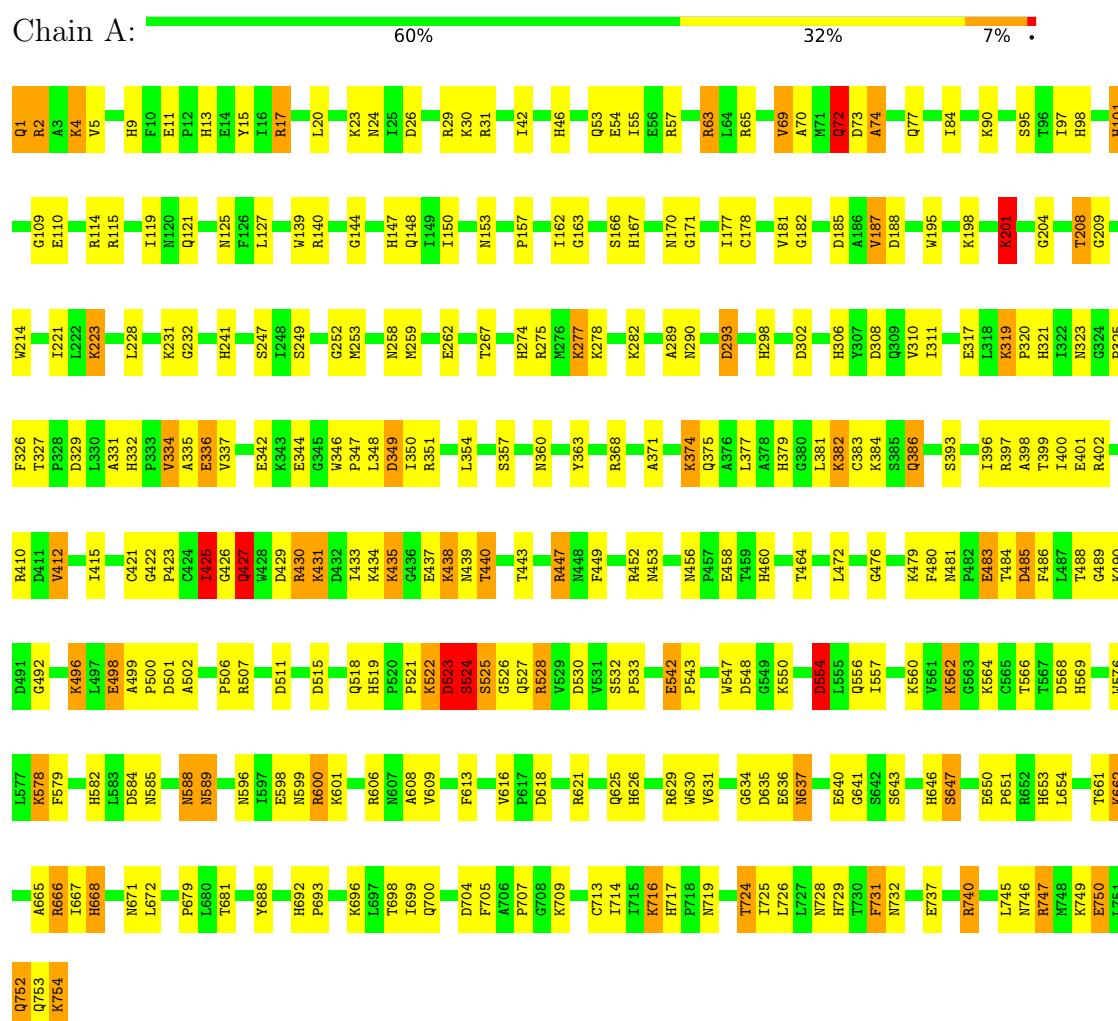
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	407	Total 407	O 407	0	0

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	173.60 Å 72.00 Å 72.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6254	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: F3S, 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	1.27	41/5943 (0.7%)	2.08	222/8053 (2.8%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	THR	CA-CB	9.26	1.64	1.53
1	A	519	HIS	CD2-NE2	-8.04	1.29	1.37
1	A	332	HIS	CD2-NE2	-7.85	1.29	1.37
1	A	167	HIS	CD2-NE2	-7.76	1.29	1.37
1	A	98	HIS	CD2-NE2	-7.38	1.29	1.37
1	A	306	HIS	CD2-NE2	-7.17	1.29	1.37
1	A	101	HIS	CD2-NE2	-7.08	1.30	1.37
1	A	241	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	668	HIS	CD2-NE2	-7.04	1.30	1.37
1	A	412	VAL	CA-CB	6.95	1.62	1.54
1	A	717	HIS	CD2-NE2	-6.89	1.30	1.37
1	A	298	HIS	CD2-NE2	-6.83	1.30	1.37
1	A	46	HIS	CD2-NE2	-6.74	1.30	1.37
1	A	460	HIS	CD2-NE2	-6.73	1.30	1.37
1	A	653	HIS	CD2-NE2	-6.70	1.30	1.37
1	A	9	HIS	CD2-NE2	-6.63	1.30	1.37
1	A	582	HIS	CD2-NE2	-6.31	1.30	1.37
1	A	147	HIS	CD2-NE2	-6.23	1.30	1.37
1	A	729	HIS	CD2-NE2	-6.19	1.31	1.37
1	A	692	HIS	CD2-NE2	-6.18	1.31	1.37
1	A	646	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	569	HIS	CG-ND1	-6.11	1.31	1.38
1	A	647	SER	CA-CB	-6.04	1.42	1.53
1	A	635	ASP	N-CA	-6.02	1.42	1.46
1	A	626	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	616	VAL	CA-CB	5.92	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	707	PRO	CA-CB	-5.87	1.45	1.53
1	A	332	HIS	CG-ND1	-5.83	1.31	1.38
1	A	321	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	569	HIS	CD2-NE2	-5.49	1.31	1.37
1	A	274	HIS	CD2-NE2	-5.47	1.31	1.37
1	A	653	HIS	CG-ND1	-5.46	1.32	1.38
1	A	98	HIS	CG-ND1	-5.40	1.32	1.38
1	A	668	HIS	CG-ND1	-5.27	1.32	1.38
1	A	464	THR	CA-CB	5.27	1.60	1.54
1	A	167	HIS	CG-ND1	-5.21	1.32	1.38
1	A	379	HIS	CD2-NE2	-5.13	1.32	1.37
1	A	460	HIS	CG-ND1	-5.09	1.32	1.38
1	A	187	VAL	CA-CB	5.05	1.61	1.54
1	A	717	HIS	CG-ND1	-5.02	1.32	1.38
1	A	740	ARG	NE-CZ	5.01	1.38	1.33

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	523	ASP	CA-CB-CG	13.84	126.44	112.60
1	A	548	ASP	CA-CB-CG	11.50	124.10	112.60
1	A	72	GLN	CA-CB-CG	10.98	136.05	114.10
1	A	72	GLN	N-CA-CB	-10.02	94.82	110.85
1	A	54	GLU	CB-CG-CD	9.98	129.56	112.60
1	A	485	ASP	N-CA-C	9.92	123.42	110.43
1	A	585	ASN	OD1-CG-ND2	-9.70	112.90	122.60
1	A	585	ASN	CB-CG-ND2	9.57	130.76	116.40
1	A	582	HIS	CB-CG-CD2	-9.45	118.91	131.20
1	A	507	ARG	N-CA-C	-9.03	101.41	111.07
1	A	447	ARG	NE-CZ-NH1	-8.95	112.55	121.50
1	A	498	GLU	CA-CB-CG	8.93	131.96	114.10
1	A	599	ASN	OD1-CG-ND2	-8.82	113.78	122.60
1	A	589	ASN	CA-CB-CG	8.81	121.41	112.60
1	A	705	PHE	CA-CB-CG	8.78	122.58	113.80
1	A	732	ASN	OD1-CG-ND2	-8.60	114.00	122.60
1	A	582	HIS	CB-CG-ND1	8.43	135.34	122.70
1	A	274	HIS	CB-CG-CD2	-8.36	120.33	131.20
1	A	425	ILE	N-CA-C	-8.25	104.54	112.29
1	A	31	ARG	N-CA-C	-8.23	101.02	112.45
1	A	167	HIS	CA-CB-CG	-8.13	105.67	113.80
1	A	692	HIS	CA-C-N	8.09	128.55	119.32
1	A	692	HIS	C-N-CA	8.09	128.55	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	666	ARG	NE-CZ-NH1	-7.98	113.52	121.50
1	A	274	HIS	CA-CB-CG	7.97	121.77	113.80
1	A	589	ASN	OD1-CG-ND2	-7.93	114.67	122.60
1	A	72	GLN	CB-CA-C	7.82	123.67	109.37
1	A	73	ASP	CA-CB-CG	7.69	120.29	112.60
1	A	447	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	A	336	GLU	N-CA-C	7.63	121.85	112.54
1	A	511	ASP	O-C-N	-7.59	114.86	121.31
1	A	170	ASN	OD1-CG-ND2	-7.56	115.04	122.60
1	A	566	THR	N-CA-CB	-7.46	100.16	110.38
1	A	589	ASN	CB-CG-ND2	7.35	127.43	116.40
1	A	440	THR	CA-CB-OG1	-7.29	98.67	109.60
1	A	542	GLU	CB-CG-CD	-7.22	100.33	112.60
1	A	241	HIS	CB-CG-CD2	-7.22	121.82	131.20
1	A	42	ILE	N-CA-C	7.07	117.86	110.72
1	A	267	THR	CA-CB-OG1	-7.04	99.05	109.60
1	A	274	HIS	CB-CG-ND1	6.97	133.16	122.70
1	A	84	ILE	CA-C-O	-6.93	113.83	121.17
1	A	368	ARG	NE-CZ-NH2	6.86	125.37	119.20
1	A	524	SER	N-CA-C	6.75	125.19	110.80
1	A	195	TRP	CG-CD1-NE1	-6.69	101.50	110.20
1	A	731	PHE	CA-CB-CG	6.69	120.49	113.80
1	A	101	HIS	CB-CG-CD2	-6.68	122.52	131.20
1	A	629	ARG	CB-CG-CD	-6.66	95.99	111.30
1	A	329	ASP	CA-CB-CG	6.64	119.24	112.60
1	A	275	ARG	NE-CZ-NH1	-6.63	114.87	121.50
1	A	140	ARG	N-CA-CB	-6.59	100.08	110.03
1	A	507	ARG	CA-CB-CG	6.59	127.28	114.10
1	A	588	ASN	OD1-CG-ND2	-6.53	116.07	122.60
1	A	247	SER	N-CA-C	-6.52	105.08	113.16
1	A	63	ARG	N-CA-CB	-6.51	99.66	110.47
1	A	500	PRO	CA-C-O	6.47	128.72	121.34
1	A	425	ILE	CB-CA-C	-6.47	103.01	111.88
1	A	662	LYS	N-CA-C	-6.47	103.73	111.69
1	A	101	HIS	CB-CG-ND1	6.46	132.38	122.70
1	A	72	GLN	CB-CG-CD	6.45	123.57	112.60
1	A	53	GLN	CG-CD-NE2	6.43	126.05	116.40
1	A	630	TRP	CG-CD2-CE3	6.42	140.32	133.90
1	A	698	THR	CA-CB-OG1	-6.38	100.04	109.60
1	A	606	ARG	NE-CZ-NH2	6.35	124.91	119.20
1	A	643	SER	N-CA-C	6.34	120.28	112.54
1	A	74	ALA	N-CA-C	-6.33	105.04	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	326	PHE	CA-CB-CG	-6.29	107.51	113.80
1	A	636	GLU	N-CA-C	6.28	120.12	110.20
1	A	732	ASN	CA-CB-CG	6.27	118.87	112.60
1	A	596	ASN	OD1-CG-ND2	-6.26	116.34	122.60
1	A	646	HIS	CB-CG-CD2	-6.24	123.08	131.20
1	A	69	VAL	O-C-N	-6.22	116.54	123.26
1	A	729	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	A	402	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	A	382	LYS	N-CA-CB	-6.17	101.82	111.56
1	A	460	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	208	THR	N-CA-CB	-6.15	100.17	111.37
1	A	125	ASN	CA-CB-CG	-6.15	106.45	112.60
1	A	110	GLU	CA-CB-CG	6.14	126.37	114.10
1	A	275	ARG	NE-CZ-NH2	6.12	124.71	119.20
1	A	427	GLN	CG-CD-NE2	6.11	125.57	116.40
1	A	323	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	527	GLN	N-CA-C	-6.10	100.62	110.32
1	A	332	HIS	CB-CG-CD2	-6.09	123.28	131.20
1	A	278	LYS	CA-CB-CG	6.09	126.28	114.10
1	A	121	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	A	150	ILE	CA-C-O	-6.06	114.75	121.17
1	A	438	LYS	N-CA-C	-6.06	99.33	108.96
1	A	386	GLN	N-CA-C	-6.05	102.54	110.53
1	A	17	ARG	NE-CZ-NH2	6.05	124.64	119.20
1	A	410	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	A	641	GLY	N-CA-C	6.03	118.87	111.45
1	A	139	TRP	CA-C-O	6.03	126.81	120.36
1	A	598	GLU	CB-CG-CD	6.01	122.81	112.60
1	A	258	ASN	OD1-CG-ND2	-6.00	116.60	122.60
1	A	483	GLU	CA-CB-CG	6.00	126.09	114.10
1	A	24	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	616	VAL	CA-C-N	5.93	125.64	119.05
1	A	616	VAL	C-N-CA	5.93	125.64	119.05
1	A	110	GLU	N-CA-C	5.92	117.73	111.28
1	A	53	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	147	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	A	46	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	A	298	HIS	CB-CG-CD2	-5.87	123.57	131.20
1	A	311	ILE	N-CA-C	-5.84	99.71	108.12
1	A	282	LYS	CB-CG-CD	5.83	124.72	111.30
1	A	290	ASN	OD1-CG-ND2	-5.83	116.77	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	GLU	N-CA-CB	-5.82	100.81	110.23
1	A	90	LYS	CA-CB-CG	5.80	125.71	114.10
1	A	481	ASN	CA-C-N	5.80	125.93	119.32
1	A	481	ASN	C-N-CA	5.80	125.93	119.32
1	A	11	GLU	O-C-N	-5.78	116.55	121.23
1	A	187	VAL	CA-C-O	-5.76	112.70	119.85
1	A	337	VAL	CA-C-O	-5.76	114.95	120.95
1	A	486	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	434	LYS	O-C-N	-5.74	116.23	123.01
1	A	5	VAL	O-C-N	-5.74	116.66	123.03
1	A	724	THR	CA-CB-OG1	-5.74	101.00	109.60
1	A	750	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	223	LYS	CG-CD-CE	5.73	124.48	111.30
1	A	729	HIS	O-C-N	-5.70	117.32	123.42
1	A	65	ARG	CA-C-N	5.66	125.61	119.78
1	A	65	ARG	C-N-CA	5.66	125.61	119.78
1	A	750	GLU	O-C-N	-5.66	114.85	122.43
1	A	195	TRP	CB-CG-CD1	-5.65	118.42	126.90
1	A	195	TRP	CE2-CD2-CG	-5.65	100.42	107.20
1	A	73	ASP	N-CA-C	5.65	119.43	112.54
1	A	447	ARG	O-C-N	-5.65	116.35	123.01
1	A	600	ARG	CA-CB-CG	5.65	125.40	114.10
1	A	667	ILE	N-CA-C	-5.64	105.02	110.72
1	A	302	ASP	CA-C-N	5.64	125.92	119.83
1	A	302	ASP	C-N-CA	5.64	125.92	119.83
1	A	699	ILE	N-CA-C	-5.64	99.62	107.80
1	A	717	HIS	CB-CG-CD2	-5.64	123.87	131.20
1	A	382	LYS	O-C-N	-5.61	116.65	123.10
1	A	298	HIS	CB-CG-ND1	5.59	131.08	122.70
1	A	157	PRO	O-C-N	-5.53	116.33	123.03
1	A	195	TRP	CD1-CG-CD2	5.53	115.14	106.30
1	A	519	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	698	THR	CA-CB-CG2	5.51	119.86	110.50
1	A	195	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	A	114	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	267	THR	CA-CB-CG2	5.50	119.85	110.50
1	A	346	TRP	CA-C-N	5.50	126.36	119.98
1	A	346	TRP	C-N-CA	5.50	126.36	119.98
1	A	201	LYS	O-C-N	-5.49	116.59	122.85
1	A	554	ASP	CA-C-O	5.49	128.36	120.51
1	A	719	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	A	334	VAL	N-CA-C	-5.46	104.27	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	484	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	348	LEU	CD1-CG-CD2	-5.45	98.82	110.80
1	A	332	HIS	CA-C-N	5.43	125.35	119.76
1	A	332	HIS	C-N-CA	5.43	125.35	119.76
1	A	410	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	A	209	GLY	CA-C-O	-5.42	113.88	122.28
1	A	383	CYS	CA-CB-SG	-5.41	101.95	114.40
1	A	530	ASP	N-CA-C	5.41	118.56	107.69
1	A	148	GLN	N-CA-C	-5.41	104.80	111.40
1	A	548	ASP	N-CA-C	5.39	119.49	113.02
1	A	728	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	57	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	634	GLY	O-C-N	5.36	128.27	123.60
1	A	588	ASN	CB-CG-ND2	5.35	124.42	116.40
1	A	542	GLU	CA-C-N	5.35	125.34	119.89
1	A	542	GLU	C-N-CA	5.35	125.34	119.89
1	A	110	GLU	CB-CG-CD	5.34	121.69	112.60
1	A	293	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	616	VAL	CA-C-O	-5.33	115.12	118.69
1	A	601	LYS	CA-CB-CG	5.32	124.74	114.10
1	A	331	ALA	N-CA-C	5.27	118.21	109.46
1	A	746	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	637	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	368	ARG	N-CA-C	-5.26	105.55	111.28
1	A	618	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	557	ILE	N-CA-C	-5.25	100.33	107.99
1	A	666	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	518	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	A	319	LYS	CA-C-N	5.21	125.13	119.76
1	A	319	LYS	C-N-CA	5.21	125.13	119.76
1	A	399	THR	O-C-N	-5.21	116.70	122.07
1	A	306	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	618	ASP	CA-C-O	-5.21	115.35	120.82
1	A	692	HIS	CB-CG-CD2	-5.21	124.42	131.20
1	A	166	SER	N-CA-C	5.20	117.69	111.71
1	A	498	GLU	CB-CA-C	5.20	118.10	109.53
1	A	502	ALA	N-CA-C	5.19	116.96	108.76
1	A	490	LYS	CA-C-N	5.19	131.27	122.65
1	A	490	LYS	C-N-CA	5.19	131.27	122.65
1	A	17	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	A	139	TRP	CE2-CD2-CE3	5.18	123.98	118.80
1	A	613	PHE	O-C-N	-5.18	116.89	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	SER	CA-CB-OG	5.17	121.44	111.10
1	A	654	LEU	N-CA-C	5.17	118.72	112.93
1	A	547	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	A	252	GLY	O-C-N	-5.16	117.24	122.19
1	A	344	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	55	ILE	N-CA-C	5.15	115.47	107.28
1	A	63	ARG	CB-CA-C	5.15	119.18	110.79
1	A	398	ALA	O-C-N	-5.15	116.73	122.09
1	A	396	ILE	N-CA-C	-5.15	105.39	111.00
1	A	740	ARG	CB-CG-CD	5.14	123.12	111.30
1	A	139	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	77	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	153	ASN	CB-CA-C	-5.08	102.52	109.28
1	A	705	PHE	N-CA-C	-5.07	102.35	109.96
1	A	560	LYS	N-CA-C	-5.07	100.26	108.52
1	A	188	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	631	VAL	CG1-CB-CG2	-5.07	99.65	110.80
1	A	576	TRP	CE2-CD2-CG	-5.07	101.12	107.20
1	A	566	THR	CA-C-O	-5.06	116.22	121.99
1	A	335	ALA	O-C-N	-5.06	116.83	122.09
1	A	460	HIS	CB-CG-ND1	5.06	130.28	122.70
1	A	427	GLN	CB-CG-CD	5.05	121.18	112.60
1	A	498	GLU	CA-C-N	5.05	127.52	120.65
1	A	498	GLU	C-N-CA	5.05	127.52	120.65
1	A	665	ALA	N-CA-C	-5.05	102.29	110.32
1	A	427	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	A	386	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	A	177	ILE	N-CA-CB	-5.03	105.13	111.41
1	A	606	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	440	THR	N-CA-CB	-5.01	102.70	110.57
1	A	140	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5823	0	5811	106	0
2	A	5	0	0	0	0
3	A	7	0	0	1	0
4	A	12	0	5	0	0
5	A	407	0	0	11	0
All	All	6254	0	5816	106	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 9.

All (106) 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	1.63	0.80
1:A:750:GLU:HA	1:A:754:LYS:HA	1.62	0.80
1:A:521:PRO:HB2	1:A:523:ASP:HB2	1.63	0.79
1:A:430:ARG:HH12	1:A:439:ASN:HD21	1.34	0.75
1:A:371:ALA:HA	1:A:374:LYS:HD3	1.68	0.75
1:A:640:GLU:HG2	5:A:970:HOH:O	1.90	0.72
1:A:447:ARG:HG3	1:A:449:PHE:HD2	1.62	0.64
1:A:431:LYS:HA	1:A:431:LYS:HE3	1.78	0.64
1:A:496:LYS:NZ	1:A:496:LYS:HB2	2.14	0.62
1:A:430:ARG:HH12	1:A:439:ASN:ND2	1.97	0.61
1:A:447:ARG:HG2	1:A:452:ARG:HG2	1.82	0.61
1:A:277:LYS:HG2	1:A:289:ALA:HB1	1.83	0.61
1:A:29:ARG:HH21	1:A:29:ARG:HG3	1.66	0.61
1:A:354:LEU:HD13	1:A:443:THR:HG22	1.82	0.60
1:A:562:LYS:O	1:A:562:LYS:HE2	2.01	0.59
1:A:374:LYS:HG2	1:A:375:GLN:N	2.18	0.58
1:A:621:ARG:O	1:A:625:GLN:HG2	2.02	0.58
1:A:737:GLU:HB3	1:A:747:ARG:HD2	1.85	0.58
1:A:182:GLY:HA3	1:A:671:ASN:HD21	1.69	0.57
1:A:754:LYS:NZ	1:A:754:LYS:HB3	2.21	0.56
1:A:745:LEU:O	1:A:749:LYS:HG3	2.06	0.56
1:A:661:THR:O	1:A:681:THR:HA	2.05	0.55
1:A:522:LYS:O	1:A:522:LYS:HD2	2.06	0.55
1:A:564:LYS:NZ	5:A:966:HOH:O	2.36	0.55
1:A:26:ASP:CG	1:A:30:LYS:HZ1	2.15	0.54
1:A:347:PRO:HD2	1:A:440:THR:OG1	2.07	0.54
1:A:221:ILE:HG12	1:A:259:MET:HB3	1.90	0.54
1:A:357:SER:HB2	3:A:999:F3S:S3	2.47	0.53
1:A:228:LEU:HB3	1:A:232:GLY:HA3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:HG3	1:A:449:PHE:CD2	2.43	0.52
1:A:351:ARG:NH1	1:A:433:ILE:HG22	2.25	0.51
1:A:672:LEU:HB2	1:A:679:PRO:HG3	1.92	0.51
1:A:1:PCA:HG3	1:A:17:ARG:HD2	1.93	0.51
1:A:427:GLN:HG2	5:A:1013:HOH:O	2.11	0.50
1:A:397:ARG:HD2	5:A:877:HOH:O	2.12	0.50
1:A:749:LYS:O	1:A:752:GLN:HG2	2.12	0.50
1:A:29:ARG:HG3	1:A:29:ARG:NH2	2.26	0.49
1:A:13:HIS:H	1:A:13:HIS:CD2	2.30	0.49
1:A:371:ALA:CA	1:A:374:LYS:HD3	2.41	0.49
1:A:498:GLU:HB2	5:A:1118:HOH:O	2.12	0.49
1:A:162:ILE:HD12	1:A:181:VAL:HG21	1.93	0.48
1:A:198:LYS:HE2	5:A:823:HOH:O	2.12	0.48
1:A:181:VAL:HB	1:A:185:ASP:HB2	1.94	0.48
1:A:479:LYS:HD2	1:A:479:LYS:HA	1.68	0.48
1:A:562:LYS:HE2	1:A:562:LYS:C	2.38	0.48
1:A:2:ARG:H	1:A:2:ARG:HD3	1.78	0.48
1:A:637:ASN:O	1:A:640:GLU:HB2	2.14	0.48
1:A:483:GLU:HA	5:A:1031:HOH:O	2.12	0.47
1:A:320:PRO:HB2	1:A:334:VAL:HG22	1.94	0.47
1:A:374:LYS:HE2	1:A:375:GLN:HG3	1.95	0.47
1:A:384:LYS:HD3	5:A:812:HOH:O	2.15	0.47
1:A:63:ARG:NH2	5:A:1172:HOH:O	2.48	0.47
1:A:320:PRO:HB2	1:A:334:VAL:CG2	2.44	0.47
1:A:662:LYS:HE3	1:A:688:TYR:CG	2.50	0.47
1:A:496:LYS:HB2	1:A:496:LYS:HZ2	1.79	0.47
1:A:72:GLN:OE1	1:A:74:ALA:HB3	2.14	0.47
1:A:204:GLY:O	1:A:310:VAL:HA	2.13	0.47
1:A:650:GLU:HB2	1:A:651:PRO:HD3	1.97	0.47
1:A:700:GLN:OE1	1:A:714:ILE:HD11	2.14	0.47
1:A:69:VAL:O	1:A:95:SER:HA	2.15	0.47
1:A:144:GLY:HA3	1:A:393:SER:HA	1.96	0.46
1:A:435:LYS:HD2	1:A:456:ASN:HA	1.97	0.46
1:A:480:PHE:CE2	1:A:485:ASP:HB2	2.50	0.46
1:A:350:ILE:CD1	1:A:472:LEU:HB3	2.45	0.46
1:A:277:LYS:HZ1	1:A:293:ASP:CG	2.23	0.46
1:A:578:LYS:HE3	1:A:579:PHE:CZ	2.51	0.46
1:A:588:ASN:OD1	1:A:621:ARG:NH1	2.48	0.46
1:A:713:CYS:HB3	1:A:725:ILE:HG13	1.98	0.46
1:A:72:GLN:HG2	1:A:101:HIS:CE1	2.51	0.45
1:A:381:LEU:HD21	1:A:489:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:GLY:HA2	1:A:453:ASN:O	2.17	0.45
1:A:679:PRO:HD2	1:A:731:PHE:CE2	2.51	0.45
1:A:704:ASP:OD1	1:A:709:LYS:NZ	2.51	0.44
1:A:422:GLY:HA3	1:A:423:PRO:HD3	1.85	0.44
1:A:363:TYR:CE1	1:A:506:PRO:HG3	2.53	0.44
1:A:171:GLY:HA3	1:A:178:CYS:SG	2.58	0.44
1:A:542:GLU:HA	1:A:543:PRO:HD3	1.87	0.44
1:A:528:ARG:HB2	5:A:919:HOH:O	2.17	0.43
1:A:351:ARG:HH12	1:A:437:GLU:CD	2.26	0.43
1:A:521:PRO:C	1:A:523:ASP:N	2.77	0.43
1:A:70:ALA:O	1:A:163:GLY:HA2	2.19	0.43
1:A:214:TRP:CE2	1:A:499:ALA:HA	2.53	0.43
1:A:349:ASP:OD2	1:A:384:LYS:NZ	2.52	0.43
1:A:524:SER:O	1:A:526:GLY:N	2.52	0.43
1:A:435:LYS:HA	1:A:435:LYS:HD3	1.75	0.43
1:A:249:SER:O	1:A:253:MET:HG3	2.19	0.42
1:A:97:ILE:HG21	1:A:127:LEU:HD13	2.01	0.42
1:A:29:ARG:HH21	1:A:29:ARG:CG	2.27	0.42
1:A:554:ASP:OD1	1:A:716:LYS:NZ	2.52	0.42
1:A:4:LYS:HG3	1:A:15:TYR:CZ	2.55	0.42
1:A:438:LYS:NZ	1:A:458:GLU:OE2	2.52	0.42
1:A:26:ASP:OD2	1:A:30:LYS:NZ	2.49	0.42
1:A:115:ARG:O	1:A:119:ILE:HG12	2.20	0.42
1:A:382:LYS:NZ	5:A:1073:HOH:O	2.52	0.42
1:A:342:GLU:CD	1:A:479:LYS:NZ	2.77	0.41
1:A:421:CYS:HB2	1:A:425:ILE:HD11	2.02	0.41
1:A:647:SER:HB3	1:A:668:HIS:CE1	2.56	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.83	0.41
1:A:400:ILE:HG13	1:A:401:GLU:N	2.36	0.41
1:A:429:ASP:OD1	1:A:431:LYS:NZ	2.54	0.41
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.92	0.41
1:A:754:LYS:HB3	1:A:754:LYS:HZ2	1.85	0.41
1:A:201:LYS:HG3	1:A:308:ASP:OD1	2.21	0.40
1:A:374:LYS:NZ	1:A:501:ASP:OD1	2.55	0.40
1:A:430:ARG:CZ	1:A:433:ILE:HG12	2.52	0.40
1:A:556:GLN:NE2	1:A:608:ALA:HB2	2.35	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	752/754 (100%)	705 (94%)	41 (6%)	6 (1%)	16	12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	A	524	SER
1	A	109	GLY
1	A	525	SER
1	A	492	GLY
1	A	554	ASP

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	622/622 (100%)	571 (92%)	51 (8%)	10	8

All (51) 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

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Mol	Chain	Res	Type
1	A	187	VAL
1	A	201	LYS
1	A	208	THR
1	A	223	LYS
1	A	262	GLU
1	A	277	LYS
1	A	317	GLU
1	A	319	LYS
1	A	325	PRO
1	A	327	THR
1	A	336	GLU
1	A	349	ASP
1	A	360	ASN
1	A	374	LYS
1	A	386	GLN
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	496	LYS
1	A	515	ASP
1	A	522	LYS
1	A	525	SER
1	A	528	ARG
1	A	533	PRO
1	A	550	LYS
1	A	562	LYS
1	A	568	ASP
1	A	578	LYS
1	A	589	ASN
1	A	600	ARG
1	A	609	VAL
1	A	666	ARG
1	A	693	PRO
1	A	696	LYS
1	A	716	LYS
1	A	724	THR
1	A	726	LEU
1	A	740	ARG

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Mol	Chain	Res	Type
1	A	747	ARG
1	A	752	GLN
1	A	753	GLN
1	A	754	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	77	GLN
1	A	125	ASN
1	A	395	GLN
1	A	439	ASN
1	A	514	GLN
1	A	589	ASN
1	A	653	HIS
1	A	671	ASN
1	A	675	GLN
1	A	722	GLN
1	A	728	ASN
1	A	746	ASN

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	1.00	0	9,10,12	1.56	2 (22%)

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.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-N	-2.58	119.38	124.96
1	A	1	PCA	CG-CD-N	2.41	114.28	108.39

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	$\# Z > 2$
2	SO4	A	998	-	4,4,4	0.74	0	6,6,6	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TRC	A	899	-	11,11,11	1.65	2 (18%)	14,14,14	1.73	4 (28%)
3	F3S	A	999	1	0,9,9	-	-	-		

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
4	TRC	A	899	-	-	2/12/12/12	-
3	F3S	A	999	1	-	-	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	899	TRC	C2-C3	2.47	1.58	1.53
4	A	899	TRC	C4-C5	2.11	1.56	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	899	TRC	C3-C4-C5	3.63	122.12	113.92
4	A	899	TRC	O4-C5-C4	3.18	123.87	114.00
4	A	899	TRC	C4-C3-C2	2.07	116.65	111.71
4	A	899	TRC	O4-C5-O3	-2.02	118.15	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	F3S	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.