



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:13 AM UTC

PDB ID : 1PNM / pdb_00001pnm
Title : PENICILLIN ACYLASE HAS A SINGLE-AMINO-ACID CATALYTIC CENTRE
Authors : Duggleby, H.J.; Moody, P.C.E.
Deposited on : 1995-03-16
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

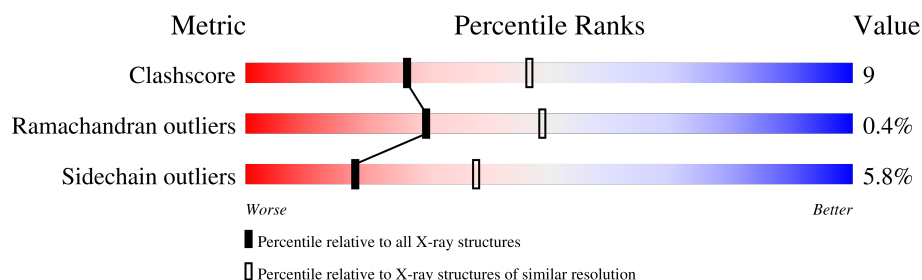
1 Overall quality at a glance

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	209	
2	B	557	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6440 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 PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1545	989	258	290	8			

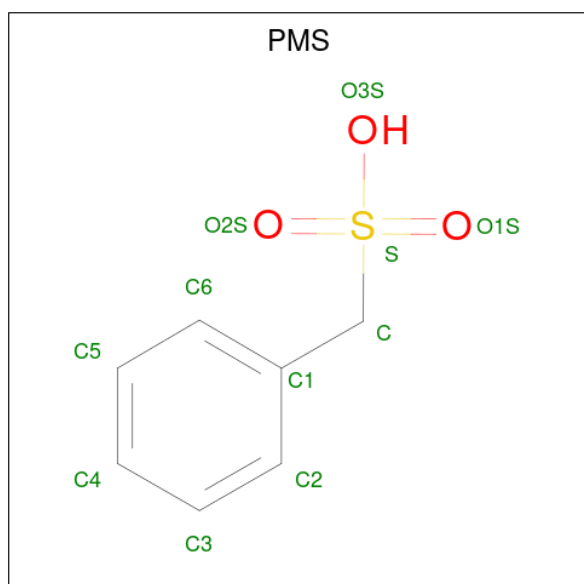
- Molecule 2 is a protein called PENICILLIN AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	0	0	0
			4415	2805	766	834	10			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

- Molecule 4 is phenylmethanesulfonic acid (CCD ID: PMS) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			10	7	2	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total	O	0	0
			120	120		
5	B	349	Total	O	0	0
			349	349		



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	52.12Å 65.08Å 76.30Å 100.20° 111.44° 105.81°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.163 , 0.222	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6440	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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: PMS, CA

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	1.05	2/1584 (0.1%)	2.36	99/2150 (4.6%)
2	B	1.06	2/4541 (0.0%)	2.37	266/6192 (4.3%)
All	All	1.06	4/6125 (0.1%)	2.37	365/8342 (4.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	25	GLY	N-CA	7.37	1.51	1.45
2	B	412	ASP	C-N	6.72	1.43	1.33
1	A	130	GLU	N-CA	5.36	1.49	1.46
1	A	109	THR	CA-CB	5.07	1.61	1.53

All (365) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	284	ASP	CA-CB-CG	-12.75	99.85	112.60
2	B	269	ARG	CA-CB-CG	11.96	138.02	114.10
2	B	391	VAL	CB-CA-C	-11.73	96.95	111.97
2	B	24	PHE	CA-CB-CG	11.46	125.26	113.80
2	B	233	GLN	CB-CG-CD	11.31	131.83	112.60
2	B	491	THR	CA-C-N	10.96	140.32	121.14
2	B	491	THR	C-N-CA	10.96	140.32	121.14
2	B	229	VAL	N-CA-CB	10.94	129.29	111.36
1	A	110	ASN	N-CA-CB	-10.82	98.48	110.71
2	B	45	THR	OG1-CB-CG2	10.80	130.91	109.30
2	B	391	VAL	N-CA-CB	10.63	122.99	110.55
1	A	150	THR	N-CA-CB	10.62	131.26	111.52
2	B	25	GLY	N-CA-C	-10.43	101.40	112.04
2	B	224	GLU	CB-CG-CD	10.22	129.97	112.60
1	A	13	GLU	CB-CG-CD	9.79	129.25	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	437	ARG	NE-CZ-NH1	9.66	131.16	121.50
2	B	269	ARG	NH1-CZ-NH2	-9.65	106.76	119.30
2	B	363	VAL	CA-C-O	9.63	125.45	119.19
2	B	269	ARG	CD-NE-CZ	9.42	137.59	124.40
2	B	301	PRO	CA-C-N	9.25	132.46	120.44
2	B	301	PRO	C-N-CA	9.25	132.46	120.44
2	B	472	HIS	CA-CB-CG	-9.22	104.58	113.80
2	B	164	GLN	CB-CG-CD	9.17	128.18	112.60
2	B	550	GLN	OE1-CD-NE2	9.05	131.65	122.60
1	A	28	PHE	CA-CB-CG	-9.04	104.76	113.80
2	B	269	ARG	N-CA-CB	8.86	124.22	109.78
2	B	496	PRO	CA-C-N	8.76	135.32	122.71
2	B	496	PRO	C-N-CA	8.76	135.32	122.71
2	B	377	GLU	CA-C-N	8.72	138.21	121.54
2	B	377	GLU	C-N-CA	8.72	138.21	121.54
2	B	533	ARG	CD-NE-CZ	8.70	136.58	124.40
2	B	467	ALA	CA-C-N	8.66	134.46	120.60
2	B	467	ALA	C-N-CA	8.66	134.46	120.60
2	B	289	THR	CA-C-N	8.47	131.63	120.28
2	B	289	THR	C-N-CA	8.47	131.63	120.28
2	B	460	PHE	CA-CB-CG	8.28	122.08	113.80
2	B	133	THR	N-CA-CB	8.21	122.46	110.47
2	B	495	ARG	CG-CD-NE	8.16	129.95	112.00
2	B	530	ASN	CA-CB-CG	8.15	120.75	112.60
2	B	331	LEU	CA-C-O	-8.12	111.32	120.66
2	B	493	SER	CA-C-O	8.12	130.61	121.51
1	A	62	PHE	CA-CB-CG	-8.03	105.77	113.80
2	B	233	GLN	CA-C-O	-8.00	111.99	120.63
1	A	117	LYS	CA-C-N	7.88	131.62	120.28
1	A	117	LYS	C-N-CA	7.88	131.62	120.28
2	B	480	GLY	CA-C-N	7.86	130.81	120.28
2	B	480	GLY	C-N-CA	7.86	130.81	120.28
2	B	83	SER	N-CA-CB	7.85	123.41	110.85
2	B	233	GLN	CA-C-N	7.84	131.56	120.28
2	B	233	GLN	C-N-CA	7.84	131.56	120.28
2	B	225	MET	CA-C-O	-7.82	109.76	119.38
1	A	38	ASP	N-CA-C	7.80	120.92	111.40
2	B	407	ILE	CA-C-O	7.77	123.47	119.12
1	A	137	ILE	N-CA-CB	7.74	119.61	110.55
1	A	194	GLU	CA-C-O	-7.71	112.96	120.90
1	A	22	ASN	CA-CB-CG	-7.71	104.89	112.60
2	B	381	ASP	CA-C-N	7.61	133.81	121.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	381	ASP	C-N-CA	7.61	133.81	121.87
1	A	105	ASP	CA-C-O	-7.58	112.86	120.82
2	B	13	ASP	CA-CB-CG	7.56	120.16	112.60
2	B	429	ASP	CA-CB-CG	7.54	120.14	112.60
1	A	136	MET	CA-C-N	7.52	130.03	120.56
1	A	136	MET	C-N-CA	7.52	130.03	120.56
2	B	414	PHE	CA-C-N	7.50	133.03	122.46
2	B	414	PHE	C-N-CA	7.50	133.03	122.46
1	A	168	VAL	N-CA-C	7.48	118.01	110.23
2	B	88	GLY	CA-C-N	7.45	134.50	122.81
2	B	88	GLY	C-N-CA	7.45	134.50	122.81
1	A	131	PRO	O-C-N	-7.43	113.69	122.24
2	B	419	GLN	OE1-CD-NE2	7.33	129.93	122.60
2	B	322	THR	CA-C-N	7.33	130.10	120.28
2	B	322	THR	C-N-CA	7.33	130.10	120.28
2	B	552	VAL	CA-C-O	7.32	128.07	120.39
2	B	75	VAL	CA-C-O	-7.28	112.64	120.36
1	A	150	THR	CB-CA-C	-7.25	94.50	109.94
2	B	272	GLU	CA-C-N	7.24	129.85	120.44
2	B	272	GLU	C-N-CA	7.24	129.85	120.44
2	B	389	ILE	CA-C-O	-7.24	112.60	120.85
2	B	386	SER	CA-C-O	7.17	130.19	121.87
2	B	183	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	90	MET	CA-C-N	7.13	129.84	120.28
1	A	90	MET	C-N-CA	7.13	129.84	120.28
2	B	317	ARG	NE-CZ-NH1	7.12	128.62	121.50
2	B	533	ARG	CA-C-O	7.07	128.66	120.75
1	A	108	ASN	CA-C-N	7.06	134.51	121.52
1	A	108	ASN	C-N-CA	7.06	134.51	121.52
1	A	128	ARG	NE-CZ-NH2	7.02	125.52	119.20
2	B	269	ARG	NE-CZ-NH1	7.02	128.52	121.50
1	A	13	GLU	CA-CB-CG	6.99	128.09	114.10
2	B	333	ASN	N-CA-C	-6.99	101.51	110.53
2	B	45	THR	N-CA-CB	6.97	123.61	111.13
2	B	133	THR	N-CA-C	-6.96	104.92	113.41
2	B	276	ARG	CD-NE-CZ	6.94	134.12	124.40
2	B	61	GLY	CA-C-N	6.94	130.51	123.16
2	B	61	GLY	C-N-CA	6.94	130.51	123.16
1	A	32	GLY	CA-C-N	6.92	129.43	120.44
1	A	32	GLY	C-N-CA	6.92	129.43	120.44
2	B	406	PRO	CA-C-N	6.91	127.30	122.60
2	B	406	PRO	C-N-CA	6.91	127.30	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	481	THR	CA-C-N	6.90	133.39	122.21
2	B	481	THR	C-N-CA	6.90	133.39	122.21
2	B	328	GLY	CA-C-O	-6.86	111.38	119.06
2	B	377	GLU	CB-CG-CD	6.86	124.25	112.60
1	A	59	GLY	CA-C-N	6.85	134.63	121.54
1	A	59	GLY	C-N-CA	6.85	134.63	121.54
1	A	131	PRO	CA-C-N	6.80	129.40	120.28
1	A	131	PRO	C-N-CA	6.80	129.40	120.28
1	A	122	PHE	CA-CB-CG	-6.80	107.00	113.80
2	B	229	VAL	CB-CA-C	-6.79	98.73	111.30
2	B	378	THR	CA-C-O	6.76	130.18	120.51
2	B	325	ARG	CA-C-N	6.76	132.09	122.09
2	B	325	ARG	C-N-CA	6.76	132.09	122.09
2	B	67	SER	N-CA-CB	-6.73	99.99	111.69
2	B	265	THR	CA-C-N	6.72	129.28	120.28
2	B	265	THR	C-N-CA	6.72	129.28	120.28
2	B	54	GLY	O-C-N	-6.68	116.67	123.35
1	A	149	SER	N-CA-C	6.67	119.45	109.25
2	B	290	SER	CB-CA-C	-6.67	99.72	110.79
2	B	276	ARG	NE-CZ-NH1	6.62	128.12	121.50
2	B	67	SER	N-CA-C	6.62	119.23	109.24
1	A	39	ARG	N-CA-C	6.57	119.28	110.88
2	B	191	VAL	CA-CB-CG2	6.54	121.52	110.40
1	A	193	GLN	OE1-CD-NE2	6.52	129.12	122.60
2	B	546	HIS	CA-CB-CG	-6.50	107.30	113.80
2	B	203	HIS	CG-CD2-NE2	6.48	113.68	107.20
2	B	241	ASN	CA-CB-CG	6.45	119.05	112.60
2	B	415	ALA	N-CA-CB	-6.41	102.45	111.62
1	A	58	LEU	CA-C-O	-6.41	111.84	119.15
2	B	83	SER	CA-CB-OG	6.39	123.88	111.10
2	B	185	ASN	CA-C-O	-6.38	111.59	119.18
2	B	336	GLY	CA-C-O	-6.36	112.11	119.80
2	B	85	GLU	CA-C-O	-6.34	114.15	121.82
2	B	479	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	A	174	VAL	CA-C-N	6.32	129.07	120.54
1	A	174	VAL	C-N-CA	6.32	129.07	120.54
1	A	130	GLU	CA-CB-CG	6.32	126.73	114.10
2	B	442	VAL	CA-C-N	6.31	130.70	120.60
2	B	442	VAL	C-N-CA	6.31	130.70	120.60
1	A	88	GLU	CB-CG-CD	6.29	123.30	112.60
2	B	131	GLN	CA-C-N	6.29	131.38	120.68
2	B	131	GLN	C-N-CA	6.29	131.38	120.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	ASP	CA-CB-CG	-6.29	106.31	112.60
2	B	153	ALA	CA-C-N	6.28	129.32	120.28
2	B	153	ALA	C-N-CA	6.28	129.32	120.28
2	B	176	THR	CA-CB-CG2	6.27	121.17	110.50
2	B	100	LEU	N-CA-C	-6.26	100.31	110.20
2	B	69	ALA	CB-CA-C	6.25	119.66	109.90
1	A	140	GLY	N-CA-C	6.22	121.39	113.24
1	A	75	PRO	CA-C-N	6.19	128.57	120.28
1	A	75	PRO	C-N-CA	6.19	128.57	120.28
2	B	216	ASP	CA-CB-CG	6.18	118.78	112.60
2	B	335	ASP	CA-CB-CG	6.18	118.78	112.60
2	B	313	SER	CA-C-N	6.15	129.81	121.20
2	B	313	SER	C-N-CA	6.15	129.81	121.20
2	B	360	VAL	CA-C-N	6.13	128.50	120.28
2	B	360	VAL	C-N-CA	6.13	128.50	120.28
2	B	161	LYS	CB-CG-CD	6.13	125.39	111.30
2	B	530	ASN	OD1-CG-ND2	6.13	128.73	122.60
2	B	556	GLN	N-CA-CB	6.12	122.08	111.00
1	A	95	GLY	CA-C-N	6.11	129.28	120.79
1	A	95	GLY	C-N-CA	6.11	129.28	120.79
2	B	245	GLN	N-CA-CB	-6.10	102.11	111.56
2	B	479	ARG	NH1-CZ-NH2	-6.09	111.38	119.30
1	A	70	ARG	CA-C-O	-6.07	114.11	120.55
1	A	71	ARG	CD-NE-CZ	6.07	132.90	124.40
2	B	54	GLY	CA-C-N	6.05	130.47	122.30
2	B	54	GLY	C-N-CA	6.05	130.47	122.30
1	A	79	ARG	CA-C-N	6.04	128.37	120.28
1	A	79	ARG	C-N-CA	6.04	128.37	120.28
2	B	269	ARG	NE-CZ-NH2	6.02	124.62	119.20
2	B	248	TYR	CA-C-O	6.01	125.11	119.76
1	A	153	ILE	CA-C-N	6.00	128.81	120.29
1	A	153	ILE	C-N-CA	6.00	128.81	120.29
2	B	437	ARG	CD-NE-CZ	5.99	132.78	124.40
2	B	229	VAL	O-C-N	5.97	130.02	123.09
1	A	137	ILE	N-CA-C	-5.95	104.71	110.42
2	B	234	SER	CB-CA-C	-5.95	99.63	110.63
2	B	123	HIS	CA-C-O	-5.94	113.64	120.24
2	B	462	VAL	CA-C-O	5.91	123.03	119.19
2	B	41	GLY	CA-C-N	5.90	131.44	122.65
2	B	41	GLY	C-N-CA	5.90	131.44	122.65
1	A	101	ASN	CA-C-N	5.90	128.99	120.79
1	A	101	ASN	C-N-CA	5.90	128.99	120.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	163	TRP	CA-C-N	5.88	128.08	120.44
2	B	163	TRP	C-N-CA	5.88	128.08	120.44
1	A	125	THR	O-C-N	5.87	126.13	121.55
1	A	106	LYS	CA-C-N	5.87	127.95	120.56
1	A	106	LYS	C-N-CA	5.87	127.95	120.56
2	B	543	VAL	CA-C-O	-5.86	114.96	121.17
2	B	376	TYR	CA-C-N	5.85	132.72	121.54
2	B	376	TYR	C-N-CA	5.85	132.72	121.54
2	B	555	VAL	O-C-N	5.84	129.35	123.10
2	B	222	PRO	CA-C-N	5.82	129.91	120.60
2	B	222	PRO	C-N-CA	5.82	129.91	120.60
2	B	529	GLU	CA-C-O	-5.82	114.67	120.90
2	B	476	TYR	N-CA-CB	5.81	118.52	109.97
2	B	269	ARG	CB-CA-C	-5.80	101.11	110.74
2	B	318	GLN	OE1-CD-NE2	5.80	128.40	122.60
2	B	1	SER	O-C-N	5.77	132.24	123.00
2	B	435	SER	CA-C-N	5.77	128.01	120.28
2	B	435	SER	C-N-CA	5.77	128.01	120.28
2	B	520	HIS	CA-CB-CG	-5.76	108.03	113.80
2	B	2	ASN	CA-CB-CG	5.75	118.35	112.60
1	A	60	LYS	CB-CA-C	-5.75	98.98	110.42
2	B	444	ASN	CB-CA-C	5.74	120.27	111.02
2	B	187	ASN	CA-C-O	-5.73	114.52	121.05
1	A	175	PHE	N-CA-CB	5.72	118.46	109.94
2	B	215	TRP	CA-CB-CG	-5.72	102.73	113.60
2	B	106	ILE	N-CA-CB	5.71	118.55	111.41
2	B	278	THR	N-CA-C	-5.71	102.31	110.59
2	B	333	ASN	OD1-CG-ND2	5.71	128.31	122.60
2	B	20	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	25	TRP	CA-C-N	5.71	128.39	120.29
1	A	25	TRP	C-N-CA	5.71	128.39	120.29
2	B	72	GLY	N-CA-C	-5.70	103.67	112.85
2	B	248	TYR	CB-CA-C	5.70	118.64	109.41
2	B	476	TYR	N-CA-C	-5.69	101.86	110.28
2	B	8	LYS	CA-C-N	5.69	130.22	120.72
2	B	8	LYS	C-N-CA	5.69	130.22	120.72
2	B	8	LYS	CB-CA-C	-5.67	101.32	110.74
1	A	107	VAL	N-CA-CB	5.67	117.18	110.55
1	A	3	SER	CA-C-O	5.67	130.44	120.80
2	B	145	GLY	CA-C-N	5.66	131.08	122.08
2	B	145	GLY	C-N-CA	5.66	131.08	122.08
2	B	70	GLY	CA-C-N	5.66	130.17	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	GLY	C-N-CA	5.66	130.17	122.19
2	B	493	SER	CA-C-N	5.65	131.61	121.66
2	B	493	SER	C-N-CA	5.65	131.61	121.66
1	A	41	PHE	CA-CB-CG	-5.64	108.16	113.80
2	B	242	ASN	OD1-CG-ND2	5.64	128.24	122.60
1	A	98	ASP	CA-C-N	5.64	126.36	119.99
1	A	98	ASP	C-N-CA	5.64	126.36	119.99
2	B	203	HIS	CE1-NE2-CD2	-5.63	103.36	109.00
2	B	378	THR	CA-C-N	5.63	129.60	122.16
2	B	378	THR	C-N-CA	5.63	129.60	122.16
2	B	322	THR	CA-CB-OG1	-5.63	101.16	109.60
1	A	29	TYR	CA-C-N	5.62	126.34	119.99
1	A	29	TYR	C-N-CA	5.62	126.34	119.99
2	B	391	VAL	CA-C-N	5.61	126.33	119.99
2	B	391	VAL	C-N-CA	5.61	126.33	119.99
2	B	245	GLN	CA-CB-CG	5.61	125.31	114.10
2	B	318	GLN	CA-C-N	5.61	128.11	120.54
2	B	318	GLN	C-N-CA	5.61	128.11	120.54
1	A	125	THR	CA-CB-CG2	5.60	120.03	110.50
2	B	110	ASN	OD1-CG-ND2	-5.58	117.02	122.60
2	B	483	ASN	N-CA-CB	5.58	120.45	110.80
2	B	83	SER	N-CA-C	-5.58	101.08	109.95
2	B	88	GLY	CA-C-O	5.58	126.69	119.44
1	A	88	GLU	N-CA-CB	5.57	118.15	110.07
2	B	468	GLU	CG-CD-OE2	-5.55	105.64	118.40
2	B	459	PHE	CA-C-N	5.54	130.84	121.14
2	B	459	PHE	C-N-CA	5.54	130.84	121.14
2	B	49	PRO	O-C-N	-5.54	116.64	123.01
2	B	425	ALA	CA-C-N	5.54	128.15	120.29
2	B	425	ALA	C-N-CA	5.54	128.15	120.29
1	A	109	THR	CA-CB-CG2	5.53	119.91	110.50
2	B	468	GLU	CB-CG-CD	5.53	122.01	112.60
2	B	176	THR	CA-CB-OG1	-5.53	101.31	109.60
2	B	76	ASP	CA-CB-CG	5.51	118.11	112.60
2	B	213	GLY	N-CA-C	5.49	126.19	113.18
2	B	311	THR	CA-C-N	5.49	128.18	120.28
2	B	311	THR	C-N-CA	5.49	128.18	120.28
2	B	363	VAL	N-CA-C	5.48	114.52	108.05
1	A	48	ARG	CA-C-N	5.46	127.86	120.44
1	A	48	ARG	C-N-CA	5.46	127.86	120.44
2	B	99	MET	O-C-N	5.46	129.13	122.96
2	B	240	TRP	N-CA-C	-5.45	103.97	110.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	291	ARG	N-CA-C	5.45	120.08	113.38
2	B	477	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	B	419	GLN	CG-CD-NE2	-5.44	108.24	116.40
2	B	233	GLN	OE1-CD-NE2	-5.42	117.17	122.60
2	B	209	VAL	N-CA-CB	5.42	118.80	111.21
2	B	516	THR	CA-C-N	5.40	128.42	120.91
2	B	516	THR	C-N-CA	5.40	128.42	120.91
1	A	144	ASN	CA-C-O	-5.39	113.43	119.79
1	A	76	ASP	CA-C-O	-5.38	114.85	120.55
2	B	484	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	17	PRO	CA-C-N	5.36	130.56	123.00
1	A	17	PRO	C-N-CA	5.36	130.56	123.00
2	B	411	VAL	N-CA-CB	5.35	120.70	111.39
2	B	556	GLN	OE1-CD-NE2	-5.34	117.26	122.60
2	B	45	THR	CA-C-O	-5.34	114.19	120.60
2	B	556	GLN	CB-CG-CD	5.33	121.66	112.60
1	A	60	LYS	CA-CB-CG	5.33	124.76	114.10
1	A	64	LYS	CB-CG-CD	5.33	123.55	111.30
1	A	158	LEU	CA-C-N	5.31	127.39	120.28
1	A	158	LEU	C-N-CA	5.31	127.39	120.28
2	B	50	PHE	CA-C-N	5.31	129.66	122.07
2	B	50	PHE	C-N-CA	5.31	129.66	122.07
2	B	454	PHE	CA-CB-CG	5.30	119.10	113.80
2	B	534	LYS	CB-CG-CD	5.29	123.47	111.30
1	A	118	GLN	OE1-CD-NE2	-5.29	117.31	122.60
2	B	153	ALA	O-C-N	-5.28	116.52	122.12
1	A	11	ARG	CD-NE-CZ	5.28	131.79	124.40
2	B	203	HIS	CA-CB-CG	5.28	119.08	113.80
2	B	298	LEU	N-CA-C	5.28	117.11	111.36
2	B	303	LEU	CA-C-N	5.28	127.62	120.44
2	B	303	LEU	C-N-CA	5.28	127.62	120.44
2	B	6	ILE	CA-C-O	5.26	125.86	120.39
2	B	45	THR	CB-CA-C	-5.26	98.71	109.38
1	A	193	GLN	N-CA-CB	5.25	118.30	110.22
2	B	448	PRO	CB-CA-C	5.23	117.79	111.46
2	B	520	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
1	A	99	GLY	CA-C-O	5.22	126.43	121.05
1	A	195	SER	CA-C-O	-5.22	111.93	120.80
2	B	54	GLY	CA-C-O	5.21	125.76	121.18
1	A	40	LEU	N-CA-C	5.20	116.64	111.07
1	A	99	GLY	CA-C-N	5.20	127.20	120.44
1	A	99	GLY	C-N-CA	5.20	127.20	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	VAL	CA-C-O	-5.20	115.00	120.57
2	B	317	ARG	CD-NE-CZ	5.20	131.68	124.40
1	A	192	VAL	CA-C-N	5.16	127.72	120.28
1	A	192	VAL	C-N-CA	5.16	127.72	120.28
1	A	37	GLN	CG-CD-NE2	-5.15	108.68	116.40
1	A	110	ASN	CA-CB-CG	5.14	117.74	112.60
2	B	334	ASP	CA-C-N	5.13	131.35	121.18
2	B	334	ASP	C-N-CA	5.13	131.35	121.18
2	B	243	SER	CA-C-N	5.13	124.44	118.85
2	B	243	SER	C-N-CA	5.13	124.44	118.85
2	B	367	PHE	CA-C-N	5.12	127.66	120.28
2	B	367	PHE	C-N-CA	5.12	127.66	120.28
2	B	412	ASP	CA-C-O	5.12	126.43	120.49
1	A	195	SER	N-CA-CB	5.11	119.18	110.50
2	B	437	ARG	NH1-CZ-NH2	-5.11	112.66	119.30
2	B	108	VAL	N-CA-C	5.11	115.20	107.75
2	B	240	TRP	CA-C-O	5.10	125.61	121.02
2	B	47	ASN	OD1-CG-ND2	5.10	127.70	122.60
2	B	550	GLN	CG-CD-NE2	-5.09	108.77	116.40
2	B	321	GLU	CA-CB-CG	-5.09	103.93	114.10
2	B	121	THR	CA-C-N	5.08	128.50	120.47
2	B	121	THR	C-N-CA	5.08	128.50	120.47
2	B	459	PHE	O-C-N	-5.08	116.27	122.22
2	B	122	VAL	CA-C-N	5.08	129.26	120.58
2	B	122	VAL	C-N-CA	5.08	129.26	120.58
2	B	404	LYS	CA-C-N	5.08	130.59	120.94
2	B	404	LYS	C-N-CA	5.08	130.59	120.94
2	B	414	PHE	CA-CB-CG	-5.08	108.72	113.80
2	B	491	THR	N-CA-C	-5.08	107.09	113.28
2	B	1	SER	CA-C-N	-5.07	114.00	122.92
2	B	1	SER	C-N-CA	-5.07	114.00	122.92
2	B	321	GLU	CG-CD-OE2	-5.07	106.74	118.40
2	B	509	GLY	N-CA-C	-5.07	106.99	115.80
1	A	112	GLU	CB-CG-CD	5.06	121.20	112.60
2	B	277	LEU	CA-C-O	5.06	126.48	120.66
2	B	271	LEU	CA-C-O	-5.06	114.16	119.97
2	B	325	ARG	CB-CG-CD	5.06	122.93	111.30
2	B	541	GLN	CA-C-O	-5.06	115.19	120.55
2	B	525	LEU	N-CA-C	5.05	116.86	111.36
1	A	26	HIS	CA-CB-CG	-5.04	108.75	113.80
2	B	509	GLY	CA-C-O	-5.04	114.45	119.04
1	A	97	ALA	CA-C-N	5.04	126.98	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ALA	C-N-CA	5.04	126.98	120.44
2	B	234	SER	N-CA-C	5.03	117.50	111.71
2	B	223	PHE	CA-C-N	5.02	127.94	120.31
2	B	223	PHE	C-N-CA	5.02	127.94	120.31
2	B	412	ASP	N-CA-C	-5.02	101.58	109.25
2	B	258	TRP	CA-C-O	-5.01	114.98	120.70
1	A	6	GLU	CA-C-O	5.01	126.40	120.69
1	A	110	ASN	OD1-CG-ND2	5.01	127.61	122.60
2	B	202	GLY	CA-C-O	5.01	125.30	119.19
2	B	339	TRP	CA-C-N	5.01	127.40	120.29
2	B	339	TRP	C-N-CA	5.01	127.40	120.29
2	B	284	ASP	CA-C-N	5.00	128.38	120.47
2	B	284	ASP	C-N-CA	5.00	128.38	120.47
2	B	497	VAL	CA-C-O	5.00	126.26	120.76

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	1545	0	1501	32	0
2	B	4415	0	4241	95	0
3	B	1	0	0	0	0
4	B	10	0	7	0	0
5	A	120	0	0	5	0
5	B	349	0	0	16	0
All	All	6440	0	5749	109	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 (109) 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)
2:B:377:GLU:HA	5:B:804:HOH:O	1.42	1.16
1:A:18:HIS:HD2	2:B:38:HIS:NE2	1.66	0.93
2:B:288:GLN:HG2	5:B:757:HOH:O	1.68	0.93
1:A:16:MET:HE1	2:B:45:THR:HG22	1.51	0.93
2:B:318:GLN:HG2	5:B:906:HOH:O	1.66	0.92
2:B:534:LYS:HE3	5:B:628:HOH:O	1.68	0.92
1:A:150:THR:HG22	2:B:252:ASP:OD2	1.76	0.85
1:A:190:ILE:HG12	2:B:229:VAL:HG22	1.61	0.81
1:A:16:MET:CE	2:B:45:THR:HG22	2.11	0.79
2:B:387:LEU:HD21	2:B:450:MET:HE1	1.64	0.79
1:A:10:VAL:HG13	2:B:547:LYS:HG3	1.64	0.79
2:B:288:GLN:CG	5:B:757:HOH:O	2.30	0.75
2:B:164:GLN:HG3	5:B:904:HOH:O	1.87	0.74
2:B:269:ARG:HH21	2:B:297:ARG:HD3	1.53	0.73
2:B:339:TRP:HH2	2:B:450:MET:HE2	1.57	0.70
1:A:150:THR:HG22	2:B:252:ASP:CG	2.17	0.70
2:B:214:LYS:H	2:B:214:LYS:HD2	1.59	0.68
1:A:56:GLU:O	2:B:109:LYS:HB2	1.94	0.67
1:A:150:THR:CG2	2:B:252:ASP:OD2	2.42	0.66
2:B:378:THR:HG22	2:B:383:PRO:HG3	1.78	0.64
2:B:106:ILE:HD11	2:B:116:PHE:HE1	1.61	0.64
1:A:60:LYS:HG3	5:B:709:HOH:O	1.96	0.63
1:A:125:THR:HB	1:A:126:PRO:HD2	1.80	0.63
2:B:378:THR:HG21	2:B:450:MET:HG2	1.82	0.62
2:B:6:ILE:HG23	2:B:10:LYS:HB3	1.81	0.61
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.82	0.61
1:A:18:HIS:CD2	2:B:38:HIS:NE2	2.58	0.61
2:B:511:ILE:HG12	2:B:517:VAL:HG22	1.83	0.60
1:A:88:GLU:CG	5:A:294:HOH:O	2.49	0.60
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.38	0.59
1:A:150:THR:HG22	2:B:252:ASP:OD1	2.02	0.58
1:A:166:TYR:O	1:A:170:GLN:HB3	2.04	0.58
1:A:16:MET:HE1	2:B:45:THR:CG2	2.32	0.56
2:B:12:GLN:HB2	2:B:276:ARG:HB3	1.88	0.56
2:B:274:LYS:HE2	5:B:704:HOH:O	2.06	0.55
1:A:21:ALA:O	2:B:39:GLY:HA3	2.06	0.55
2:B:312:GLN:HG3	5:B:888:HOH:O	2.07	0.54
2:B:121:THR:HG23	2:B:126:ILE:HD11	1.89	0.54
2:B:129:THR:HA	2:B:136:ALA:HA	1.91	0.53
2:B:501:ASP:OD1	2:B:534:LYS:HE2	2.09	0.53
1:A:26:HIS:HE1	2:B:556:GLN:NE2	2.07	0.52
2:B:3:MET:HE3	2:B:180:TYR:HB2	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ARG:HH21	2:B:297:ARG:CD	2.22	0.52
2:B:326:TRP:CD1	2:B:341:GLN:HG3	2.44	0.52
2:B:269:ARG:NH2	2:B:297:ARG:HB2	2.25	0.51
1:A:57:VAL:HG12	5:A:322:HOH:O	2.11	0.51
2:B:214:LYS:HD2	2:B:214:LYS:N	2.24	0.50
2:B:397:TYR:O	2:B:401:GLN:HG2	2.11	0.49
2:B:382:GLY:HA3	2:B:451:ALA:O	2.13	0.48
2:B:341:GLN:HG2	5:B:663:HOH:O	2.12	0.48
2:B:504:ALA:HA	2:B:505:PRO:C	2.38	0.48
2:B:104:GLU:O	2:B:115:THR:HA	2.13	0.48
2:B:197:PRO:HB3	2:B:217:TRP:CD2	2.48	0.48
1:A:88:GLU:HG2	5:A:294:HOH:O	2.13	0.48
2:B:42:TYR:CZ	2:B:159:LYS:HE3	2.49	0.48
2:B:534:LYS:NZ	5:B:644:HOH:O	2.47	0.48
2:B:378:THR:HG21	2:B:450:MET:SD	2.54	0.48
2:B:520:HIS:HE1	2:B:548:GLU:OE2	1.98	0.47
1:A:166:TYR:HB3	1:A:170:GLN:CG	2.45	0.47
2:B:401:GLN:HB2	2:B:405:SER:HB2	1.96	0.47
2:B:483:ASN:O	2:B:501:ASP:HA	2.15	0.47
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.50	0.47
1:A:88:GLU:HG3	5:A:294:HOH:O	2.13	0.46
2:B:274:LYS:CE	5:B:704:HOH:O	2.61	0.46
1:A:110:ASN:N	1:A:111:PRO:HD3	2.29	0.46
2:B:82:LEU:HD11	2:B:136:ALA:HB2	1.98	0.46
2:B:318:GLN:HA	5:B:906:HOH:O	2.15	0.46
1:A:60:LYS:CG	5:B:709:HOH:O	2.59	0.46
1:A:158:LEU:HD13	2:B:367:PHE:HB3	1.97	0.46
1:A:187:PRO:HG2	2:B:262:ASP:HB3	1.98	0.46
2:B:274:LYS:NZ	5:B:704:HOH:O	2.36	0.46
2:B:85:GLU:O	2:B:86:LYS:C	2.58	0.46
2:B:163:TRP:CZ3	2:B:189:GLY:HA3	2.51	0.46
2:B:164:GLN:HG3	2:B:164:GLN:H	1.51	0.45
2:B:326:TRP:CZ3	2:B:343:GLY:HA3	2.51	0.45
1:A:139:VAL:HG22	2:B:147:GLU:HB3	1.98	0.45
2:B:378:THR:HG21	2:B:450:MET:CG	2.47	0.45
1:A:194:GLU:O	1:A:195:SER:HB3	2.16	0.45
2:B:269:ARG:NH2	2:B:297:ARG:HD3	2.27	0.45
2:B:210:PRO:HD2	2:B:215:TRP:CD1	2.51	0.45
2:B:280:ASP:O	2:B:284:ASP:HB2	2.17	0.45
2:B:520:HIS:HD2	2:B:523:ASP:OD2	1.99	0.45
1:A:20:TYR:HA	2:B:38:HIS:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HA	1:A:116:PRO:HD3	1.91	0.45
2:B:31:TYR:CE2	2:B:49:PRO:HB3	2.53	0.44
2:B:287:ARG:NH1	5:B:757:HOH:O	2.50	0.44
2:B:8:LYS:HG3	2:B:186:GLY:HA3	2.00	0.44
2:B:348:ASN:ND2	2:B:374:SER:OG	2.50	0.44
1:A:166:TYR:HB3	1:A:170:GLN:HG3	2.00	0.44
2:B:494:ASP:OD1	2:B:495:ARG:HG3	2.17	0.44
2:B:131:GLN:H	2:B:131:GLN:HG3	1.64	0.43
2:B:80:GLU:OE2	2:B:123:HIS:ND1	2.51	0.43
2:B:106:ILE:HD11	2:B:116:PHE:CE1	2.49	0.43
2:B:383:PRO:HD2	2:B:476:TYR:CD1	2.53	0.43
2:B:468:GLU:H	2:B:468:GLU:HG3	1.46	0.43
2:B:48:THR:HA	2:B:49:PRO:HD3	1.96	0.43
2:B:129:THR:HG22	2:B:136:ALA:CB	2.48	0.43
1:A:79:ARG:NE	5:A:307:HOH:O	2.47	0.43
2:B:35:ILE:HG23	2:B:55:LEU:HD11	2.00	0.43
2:B:360:VAL:HG13	2:B:368:ASP:HB2	2.02	0.42
2:B:53:PRO:HD2	2:B:151:LEU:HD21	2.01	0.42
2:B:3:MET:HE1	2:B:66:GLY:HA3	2.02	0.41
2:B:495:ARG:HH12	2:B:537:TRP:HZ3	1.68	0.41
2:B:65:TRP:HA	2:B:180:TYR:O	2.20	0.41
2:B:387:LEU:HD22	2:B:476:TYR:CE2	2.55	0.41
2:B:508:SER:O	2:B:521:TYR:HA	2.21	0.41
2:B:284:ASP:OD2	2:B:287:ARG:NH2	2.54	0.41
2:B:310:LEU:HD13	2:B:314:ASP:OD2	2.21	0.40
2:B:207:LEU:HA	2:B:208:PRO:HD3	1.92	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	191/209 (91%)	189 (99%)	2 (1%)	0	100	100
2	B	555/557 (100%)	537 (97%)	15 (3%)	3 (0%)	24	43
All	All	746/766 (97%)	726 (97%)	17 (2%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	377	GLU
2	B	378	THR
2	B	134	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	165/180 (92%)	157 (95%)	8 (5%)	23	46
2	B	460/460 (100%)	432 (94%)	28 (6%)	17	35
All	All	625/640 (98%)	589 (94%)	36 (6%)	18	38

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	88	GLU
1	A	109	THR
1	A	112	GLU
1	A	130	GLU
1	A	150	THR
1	A	181	LEU
1	A	192	VAL
2	B	2	ASN
2	B	10	LYS
2	B	45	THR
2	B	67	SER
2	B	77	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	85	GLU
2	B	115	THR
2	B	131	GLN
2	B	133	THR
2	B	151	LEU
2	B	154	TRP
2	B	184	VAL
2	B	201	SER
2	B	214	LYS
2	B	229	VAL
2	B	317	ARG
2	B	337	LYS
2	B	366	PRO
2	B	369	LYS
2	B	378	THR
2	B	387	LEU
2	B	391	VAL
2	B	444	ASN
2	B	452	LEU
2	B	468	GLU
2	B	517	VAL
2	B	519	LYS
2	B	530	ASN

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	18	HIS
1	A	110	ASN
2	B	2	ASN
2	B	93	ASN
2	B	110	ASN
2	B	134	GLN
2	B	233	GLN
2	B	245	GLN
2	B	288	GLN
2	B	295	ASN
2	B	348	ASN
2	B	380	GLN
2	B	440	ASN
2	B	441	ASN
2	B	444	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	520	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	PMS	B	559	2	7,10,11	0.65	0	11,12,15	2.96	8 (72%)

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	PMS	B	559	2	-	2/4/4/5	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	559	PMS	C6-C1-C2	4.39	124.76	118.23
4	B	559	PMS	C4-C5-C6	-4.01	115.29	120.24
4	B	559	PMS	C5-C4-C3	3.73	124.97	119.87
4	B	559	PMS	C-C1-C6	-3.45	116.80	120.56
4	B	559	PMS	O1S-S-C	-3.29	99.88	105.55
4	B	559	PMS	C3-C2-C1	-2.78	116.71	120.61
4	B	559	PMS	O2S-S-C	2.68	110.19	105.55
4	B	559	PMS	C-C1-C2	-2.20	118.16	120.56

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	559	PMS	C1-C-S-O2S
4	B	559	PMS	C1-C-S-O1S

There are no ring outliers.

No monomer is involved in short contacts.

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.