



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 09:34 PM UTC

PDB ID : 4H67 / pdb_00004h67
Title : Crystal structure of HMP synthase Thi5 from *S. cerevisiae*
Authors : Coquille, S.C.; Roux, C.; Fitzpatrick, T.; Thore, S.
Deposited on : 2012-09-19
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

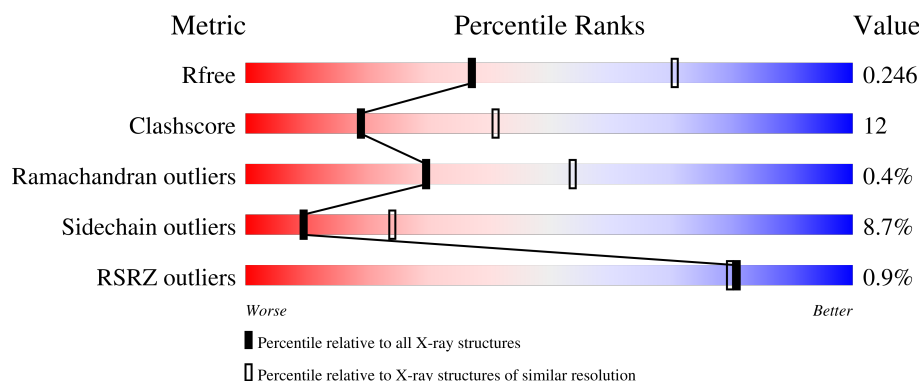
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	346	% 71% 21% 5% .
1	B	346	68% 16% . . 11%
1	C	346	4% 70% 22% 5% ..
1	D	346	% 73% 18% 5% .
1	E	346	66% 18% . 12%

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Mol	Chain	Length	Quality of chain
1	F	346	
1	G	346	
1	H	346	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	403	-	-	X	-
2	SO4	C	406	-	-	X	-
2	SO4	D	403	-	-	X	-
2	SO4	G	402	-	-	X	-
2	SO4	H	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20928 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 Pyrimidine precursor biosynthesis enzyme THI5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2701	1741	450	494	16			
1	B	307	Total	C	N	O	S	0	0	0
			2457	1592	399	452	14			
1	C	338	Total	C	N	O	S	0	0	0
			2696	1736	449	494	17			
1	D	335	Total	C	N	O	S	0	0	0
			2668	1720	438	492	18			
1	E	305	Total	C	N	O	S	0	0	0
			2440	1580	396	449	15			
1	F	335	Total	C	N	O	S	0	0	0
			2668	1720	438	492	18			
1	G	326	Total	C	N	O	S	0	0	0
			2609	1682	428	483	16			
1	H	305	Total	C	N	O	S	0	0	0
			2440	1580	396	450	14			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	SER	LYS	engineered mutation	UNP P43534
A	241	GLY	GLU	engineered mutation	UNP P43534
A	317	THR	GLN	engineered mutation	UNP P43534
A	341	HIS	-	expression tag	UNP P43534
A	342	HIS	-	expression tag	UNP P43534
A	343	HIS	-	expression tag	UNP P43534
A	344	HIS	-	expression tag	UNP P43534
A	345	HIS	-	expression tag	UNP P43534
A	346	HIS	-	expression tag	UNP P43534
B	240	SER	LYS	engineered mutation	UNP P43534
B	241	GLY	GLU	engineered mutation	UNP P43534
B	317	THR	GLN	engineered mutation	UNP P43534
B	341	HIS	-	expression tag	UNP P43534

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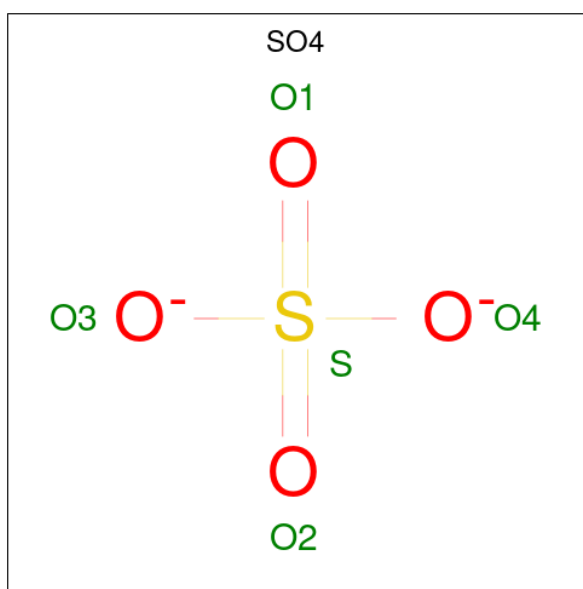
Chain	Residue	Modelled	Actual	Comment	Reference
B	342	HIS	-	expression tag	UNP P43534
B	343	HIS	-	expression tag	UNP P43534
B	344	HIS	-	expression tag	UNP P43534
B	345	HIS	-	expression tag	UNP P43534
B	346	HIS	-	expression tag	UNP P43534
C	240	SER	LYS	engineered mutation	UNP P43534
C	241	GLY	GLU	engineered mutation	UNP P43534
C	317	THR	GLN	engineered mutation	UNP P43534
C	341	HIS	-	expression tag	UNP P43534
C	342	HIS	-	expression tag	UNP P43534
C	343	HIS	-	expression tag	UNP P43534
C	344	HIS	-	expression tag	UNP P43534
C	345	HIS	-	expression tag	UNP P43534
C	346	HIS	-	expression tag	UNP P43534
D	240	SER	LYS	engineered mutation	UNP P43534
D	241	GLY	GLU	engineered mutation	UNP P43534
D	317	THR	GLN	engineered mutation	UNP P43534
D	341	HIS	-	expression tag	UNP P43534
D	342	HIS	-	expression tag	UNP P43534
D	343	HIS	-	expression tag	UNP P43534
D	344	HIS	-	expression tag	UNP P43534
D	345	HIS	-	expression tag	UNP P43534
D	346	HIS	-	expression tag	UNP P43534
E	240	SER	LYS	engineered mutation	UNP P43534
E	241	GLY	GLU	engineered mutation	UNP P43534
E	317	THR	GLN	engineered mutation	UNP P43534
E	341	HIS	-	expression tag	UNP P43534
E	342	HIS	-	expression tag	UNP P43534
E	343	HIS	-	expression tag	UNP P43534
E	344	HIS	-	expression tag	UNP P43534
E	345	HIS	-	expression tag	UNP P43534
E	346	HIS	-	expression tag	UNP P43534
F	240	SER	LYS	engineered mutation	UNP P43534
F	241	GLY	GLU	engineered mutation	UNP P43534
F	317	THR	GLN	engineered mutation	UNP P43534
F	341	HIS	-	expression tag	UNP P43534
F	342	HIS	-	expression tag	UNP P43534
F	343	HIS	-	expression tag	UNP P43534
F	344	HIS	-	expression tag	UNP P43534
F	345	HIS	-	expression tag	UNP P43534
F	346	HIS	-	expression tag	UNP P43534
G	240	SER	LYS	engineered mutation	UNP P43534

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Chain	Residue	Modelled	Actual	Comment	Reference
G	241	GLY	GLU	engineered mutation	UNP P43534
G	317	THR	GLN	engineered mutation	UNP P43534
G	341	HIS	-	expression tag	UNP P43534
G	342	HIS	-	expression tag	UNP P43534
G	343	HIS	-	expression tag	UNP P43534
G	344	HIS	-	expression tag	UNP P43534
G	345	HIS	-	expression tag	UNP P43534
G	346	HIS	-	expression tag	UNP P43534
H	240	SER	LYS	engineered mutation	UNP P43534
H	241	GLY	GLU	engineered mutation	UNP P43534
H	317	THR	GLN	engineered mutation	UNP P43534
H	341	HIS	-	expression tag	UNP P43534
H	342	HIS	-	expression tag	UNP P43534
H	343	HIS	-	expression tag	UNP P43534
H	344	HIS	-	expression tag	UNP P43534
H	345	HIS	-	expression tag	UNP P43534
H	346	HIS	-	expression tag	UNP P43534

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



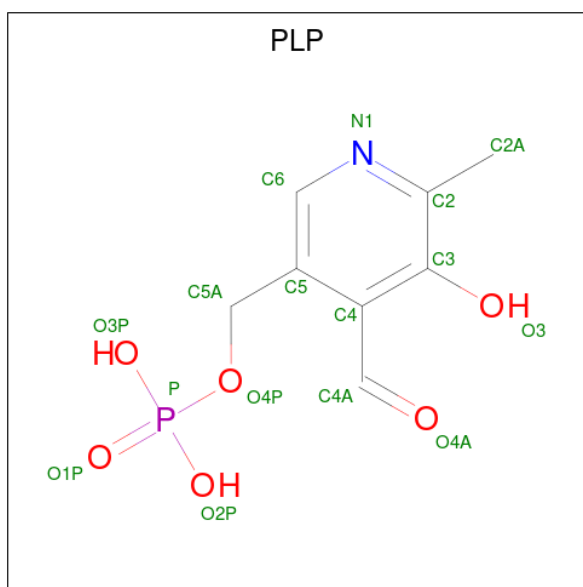
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is water.

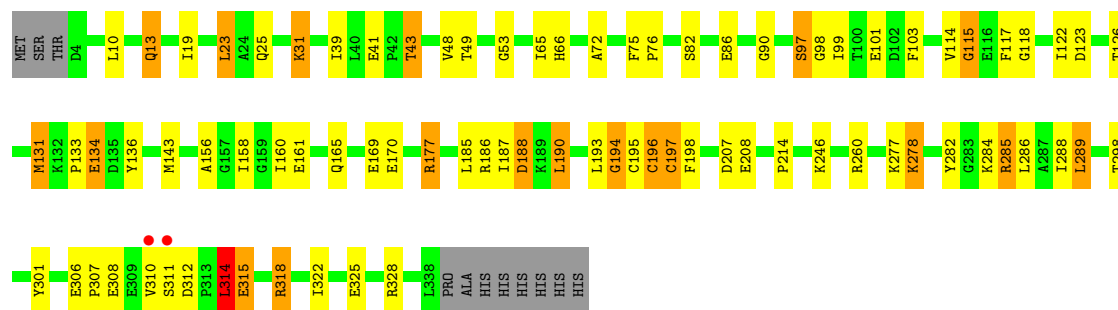
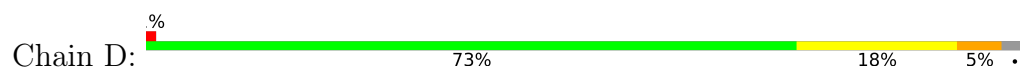
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	20	Total	O	0	0
			20	20		
4	C	25	Total	O	0	0
			25	25		
4	D	15	Total	O	0	0
			15	15		
4	E	14	Total	O	0	0
			14	14		
4	F	14	Total	O	0	0
			14	14		
4	G	13	Total	O	0	0
			13	13		
4	H	17	Total	O	0	0
			17	17		

- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

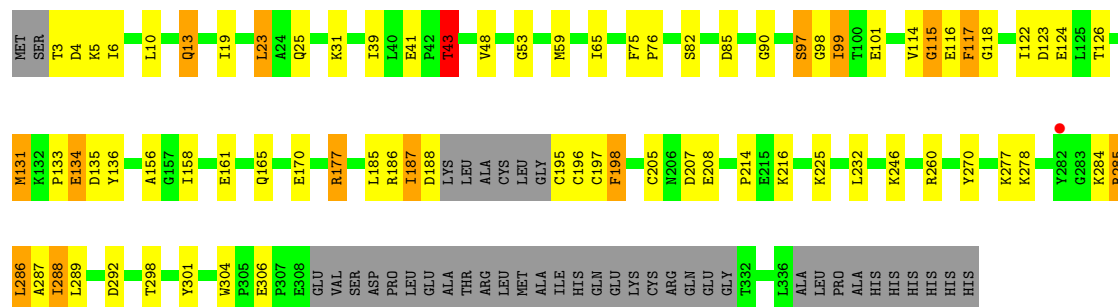




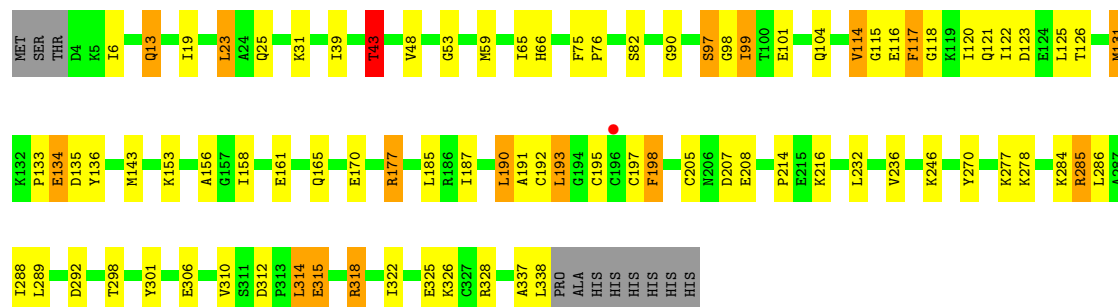
- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5



- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

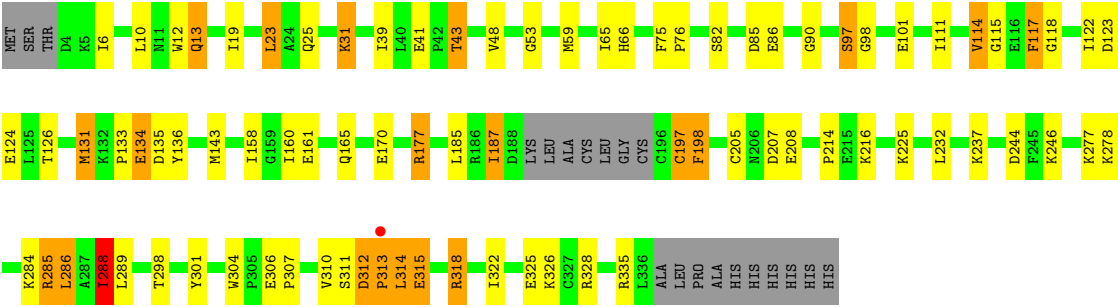


- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5

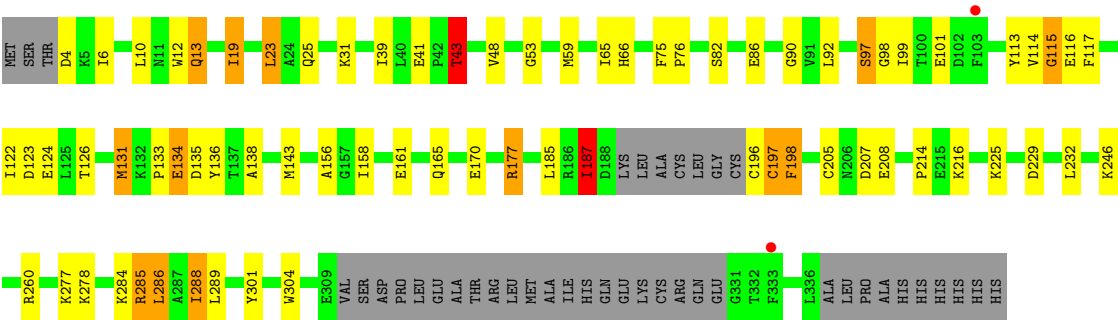


- Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5





● Molecule 1: Pyrimidine precursor biosynthesis enzyme THI5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.79Å 188.46Å 101.67Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	49.14 – 2.70 49.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.14-2.70) 95.3 (49.14-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.207 , 0.247 0.206 , 0.246	Depositor DCC
R_{free} test set	2010 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20928	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: PLP, SO4

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	0.81	1/2768 (0.0%)	0.99	11/3739 (0.3%)
1	B	0.74	0/2515	1.03	10/3394 (0.3%)
1	C	0.75	0/2761	1.01	12/3730 (0.3%)
1	D	0.72	0/2730	1.00	9/3687 (0.2%)
1	E	0.67	0/2498	0.99	9/3373 (0.3%)
1	F	0.67	1/2730 (0.0%)	0.98	9/3687 (0.2%)
1	G	0.66	0/2670	0.95	8/3605 (0.2%)
1	H	0.67	1/2498 (0.0%)	0.93	6/3372 (0.2%)
All	All	0.71	3/21170 (0.0%)	0.99	74/28587 (0.3%)

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	G	0	1
1	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	19	ILE	CA-C	6.03	1.59	1.52
1	A	312	ASP	CA-C	-5.84	1.49	1.53
1	F	114	VAL	CA-CB	-5.41	1.47	1.54

The worst 5 of 74 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	ARG	NE-CZ-NH2	13.02	130.92	119.20
1	B	274	ARG	NE-CZ-NH1	-12.71	108.79	121.50
1	E	114	VAL	N-CA-C	11.74	121.56	110.53
1	H	114	VAL	N-CA-C	11.11	121.09	110.42
1	D	114	VAL	N-CA-C	10.80	120.69	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	288	ILE	Peptide
1	H	187	ILE	Peptide

5.2 Too-close contacts [i](#)

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	2701	0	2699	79	3
1	B	2457	0	2466	53	0
1	C	2696	0	2702	87	1
1	D	2668	0	2684	70	1
1	E	2440	0	2446	52	1
1	F	2668	0	2684	60	0
1	G	2609	0	2614	66	0
1	H	2440	0	2444	46	0
2	A	15	0	0	3	0
2	C	30	0	0	6	0
2	D	15	0	0	3	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	10	0	0	3	0
2	H	5	0	0	2	0
3	B	15	0	6	5	0
4	A	31	0	0	1	0
4	B	20	0	0	2	0
4	C	25	0	0	5	0
4	D	15	0	0	1	0
4	E	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	14	0	0	1	0
4	G	13	0	0	1	0
4	H	17	0	0	3	0
All	All	20928	0	20745	491	3

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 12.

The worst 5 of 491 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:312:ASP:HB3	1:A:315:GLU:CB	1.64	1.27
1:A:274:ARG:NH2	1:A:310:VAL:HG11	1.58	1.16
1:D:118:GLY:N	2:D:403:SO4:O4	1.77	1.15
1:C:193:LEU:CG	1:C:194:GLY:H	1.55	1.13
1:C:115:GLY:N	2:C:406:SO4:O2	1.82	1.10

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ARG:NH1	1:D:314:LEU:CD2[1_455]	1.41	0.79
1:A:218:ARG:NH1	1:E:292:ASP:OD2[1_455]	1.94	0.26
1:A:96:GLY:O	1:C:107:LYS:O[2_656]	2.11	0.09

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	333/346 (96%)	324 (97%)	8 (2%)	1 (0%)	36 60
1	B	301/346 (87%)	290 (96%)	9 (3%)	2 (1%)	18 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	334/346 (96%)	320 (96%)	14 (4%)	0	100	100
1	D	333/346 (96%)	323 (97%)	9 (3%)	1 (0%)	36	60
1	E	299/346 (86%)	290 (97%)	7 (2%)	2 (1%)	18	41
1	F	333/346 (96%)	322 (97%)	11 (3%)	0	100	100
1	G	322/346 (93%)	312 (97%)	7 (2%)	3 (1%)	14	35
1	H	299/346 (86%)	286 (96%)	11 (4%)	2 (1%)	18	41
All	All	2554/2768 (92%)	2467 (97%)	76 (3%)	11 (0%)	30	54

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	GLY
1	B	115	GLY
1	E	115	GLY
1	B	187	ILE
1	G	115	GLY

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	291/298 (98%)	262 (90%)	29 (10%)	7	19
1	B	265/298 (89%)	243 (92%)	22 (8%)	10	26
1	C	291/298 (98%)	265 (91%)	26 (9%)	9	23
1	D	288/298 (97%)	263 (91%)	25 (9%)	9	24
1	E	264/298 (89%)	244 (92%)	20 (8%)	12	30
1	F	288/298 (97%)	262 (91%)	26 (9%)	9	23
1	G	282/298 (95%)	255 (90%)	27 (10%)	8	20
1	H	263/298 (88%)	244 (93%)	19 (7%)	13	32
All	All	2232/2384 (94%)	2038 (91%)	194 (9%)	9	24

5 of 194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	197	CYS
1	F	298	THR
1	E	285	ARG
1	F	131	MET
1	G	25	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	104	GLN
1	H	104	GLN
1	F	248	GLN
1	H	271	ASN
1	G	271	ASN

5.3.3 RNA [i](#)

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](#)

18 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	C	401	-	4,4,4	0.34	0	6,6,6	0.65	0
2	SO4	D	402	-	4,4,4	0.31	0	6,6,6	0.45	0
2	SO4	C	406	-	4,4,4	0.51	0	6,6,6	0.82	0
2	SO4	C	405	-	4,4,4	0.29	0	6,6,6	0.29	0
2	SO4	E	401	-	4,4,4	0.46	0	6,6,6	0.66	0
3	PLP	B	400	1	15,15,16	1.93	4 (26%)	21,22,23	2.19	7 (33%)
2	SO4	G	401	-	4,4,4	0.23	0	6,6,6	0.28	0
2	SO4	A	402	-	4,4,4	0.32	0	6,6,6	0.41	0
2	SO4	C	402	-	4,4,4	0.22	0	6,6,6	0.29	0
2	SO4	H	401	-	4,4,4	1.90	1 (25%)	6,6,6	0.88	0
2	SO4	C	403	-	4,4,4	0.40	0	6,6,6	0.39	0
2	SO4	A	403	-	4,4,4	0.54	0	6,6,6	0.55	0
2	SO4	C	404	-	4,4,4	0.33	0	6,6,6	0.27	0
2	SO4	D	401	-	4,4,4	0.26	0	6,6,6	0.27	0
2	SO4	G	402	-	4,4,4	0.56	0	6,6,6	0.38	0
2	SO4	D	403	-	4,4,4	0.55	0	6,6,6	0.64	0
2	SO4	A	401	-	4,4,4	0.22	0	6,6,6	0.64	0
2	SO4	F	401	-	4,4,4	0.54	0	6,6,6	0.58	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
3	PLP	B	400	1	-	3/6/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	PLP	O3-C3	-5.21	1.25	1.36
3	B	400	PLP	C2-N1	2.71	1.38	1.33
2	H	401	SO4	O2-S	2.29	1.58	1.44
3	B	400	PLP	C3-C4	2.27	1.44	1.40
3	B	400	PLP	P-O3P	-2.20	1.46	1.54

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	PLP	C4A-C4-C5	-6.79	113.94	120.94
3	B	400	PLP	C4A-C4-C3	3.68	126.66	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	400	PLP	C2A-C2-C3	2.52	123.75	120.80
3	B	400	PLP	O3-C3-C4	2.47	124.54	118.10
3	B	400	PLP	O2P-P-O1P	2.24	119.56	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400	PLP	C5A-O4P-P-O1P
3	B	400	PLP	C5A-O4P-P-O2P
3	B	400	PLP	C5A-O4P-P-O3P

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	406	SO4	4	0
2	E	401	SO4	1	0
3	B	400	PLP	5	0
2	G	401	SO4	1	0
2	C	402	SO4	1	0
2	H	401	SO4	2	0
2	A	403	SO4	3	0
2	C	404	SO4	1	0
2	G	402	SO4	2	0
2	D	403	SO4	3	0
2	F	401	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	337/346 (97%)	-0.00	3 (0%) 81 80	41, 65, 118, 135	0
1	B	307/346 (88%)	-0.01	1 (0%) 90 89	40, 64, 113, 138	0
1	C	338/346 (97%)	0.19	13 (3%) 44 40	43, 66, 123, 142	0
1	D	335/346 (96%)	-0.03	2 (0%) 85 85	42, 65, 124, 135	0
1	E	305/346 (88%)	-0.06	1 (0%) 90 89	41, 66, 113, 134	0
1	F	335/346 (96%)	-0.09	1 (0%) 90 89	44, 67, 126, 144	0
1	G	326/346 (94%)	-0.08	1 (0%) 90 89	40, 68, 126, 143	0
1	H	305/346 (88%)	0.06	2 (0%) 84 83	45, 68, 115, 136	0
All	All	2588/2768 (93%)	-0.00	24 (0%) 81 80	40, 66, 122, 144	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	310	VAL	3.5
1	C	185	LEU	3.5
1	C	310	VAL	3.3
1	B	333	PHE	2.9
1	A	98	GLY	2.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	C	403	5/5	0.75	0.09	91,95,140,159	0
3	PLP	B	400	15/16	0.75	0.14	56,81,103,112	0
2	SO4	C	405	5/5	0.77	0.09	102,106,139,147	0
2	SO4	A	402	5/5	0.79	0.10	65,109,111,125	0
2	SO4	C	406	5/5	0.82	0.13	85,95,107,115	0
2	SO4	C	404	5/5	0.83	0.10	60,87,142,158	0
2	SO4	G	402	5/5	0.88	0.11	68,88,95,111	0
2	SO4	D	401	5/5	0.89	0.07	74,86,112,122	0
2	SO4	F	401	5/5	0.89	0.10	66,75,111,112	0
2	SO4	A	403	5/5	0.89	0.09	77,80,93,100	0
2	SO4	C	401	5/5	0.89	0.09	59,92,104,110	0
2	SO4	D	403	5/5	0.90	0.10	61,73,105,132	0
2	SO4	A	401	5/5	0.92	0.12	55,66,77,103	0
2	SO4	D	402	5/5	0.92	0.07	68,70,85,92	0
2	SO4	E	401	5/5	0.93	0.10	54,96,118,118	0
2	SO4	G	401	5/5	0.93	0.07	51,95,108,113	0
2	SO4	H	401	5/5	0.94	0.07	85,87,96,99	0
2	SO4	C	402	5/5	0.95	0.07	54,55,80,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.