



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:36 AM UTC

PDB ID : 1UBS / pdb_00001ubs
Title : TRYPTOPHAN SYNTHASE (E.C.4.2.1.20) WITH A MUTATION OF LYS 87->THR IN THE B SUBUNIT AND IN THE PRESENCE OF LIGAND L-SERINE
Authors : Rhee, S.; Parris, K.; Ahmed, S.A.; Miles, E.W.; Davies, D.R.
Deposited on : 1995-12-14
Resolution : 1.90 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) : 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

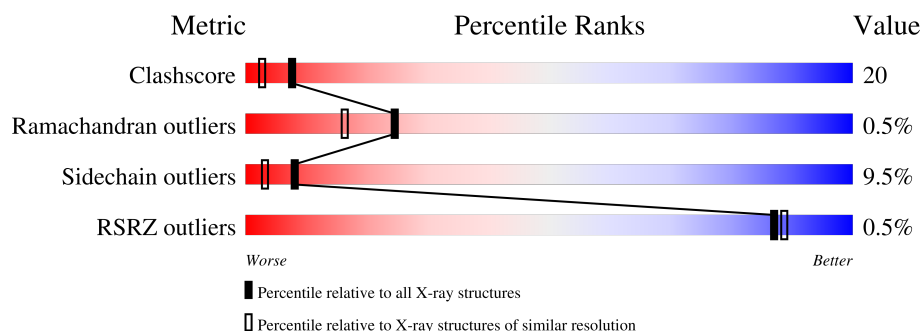
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	268	51% 34% 10% • •
2	B	397	53% 35% 10% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5184 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 TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	1	0
			1945	1235	338	364	8			

- Molecule 2 is a protein called TRYPTOPHAN SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	4	0
			2962	1863	520	560	19			

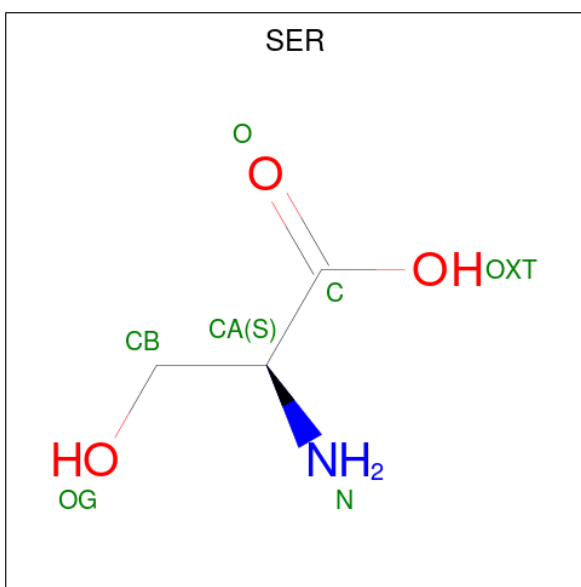
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	87	THR	LYS	engineered mutation	UNP P00933
B	396	LEU	GLU	conflict	UNP P00933

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

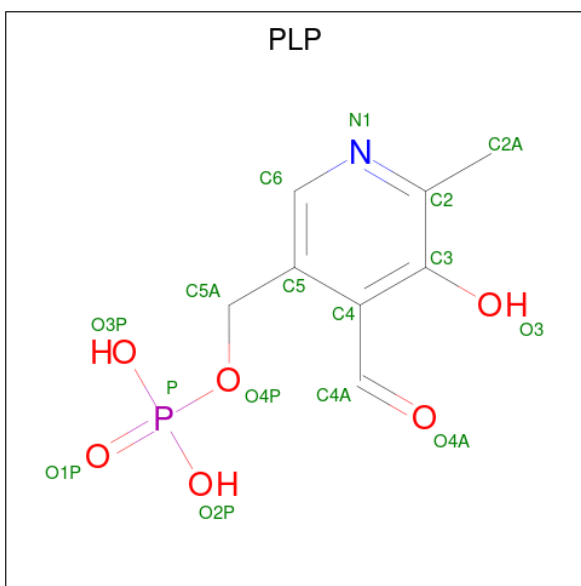
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is SERINE (CCD ID: SER) (formula: C₃H₇NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			7	3	1	3		

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	83	Total 83	O 83	0	0
6	B	171	Total 171	O 171	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

[illegible]

Chain B:

53% 35% 10%

Amino Acid	Percentage
Met	1.0%
Thr	1.0%
T3	1.0%
N6	1.0%
P7	1.0%
Y8	1.0%
F12	1.0%
G13	1.0%
Y16	1.0%
V17	1.0%
P18	1.0%
M22	1.0%
P23	1.0%
M26	1.0%
Q27	1.0%
L28	1.0%
E29	1.0%
E30	1.0%
A31	1.0%
F32	1.0%
V33	1.0%
R34	1.0%
A35	1.0%
P38	1.0%
F39	1.0%
E40	1.0%
F41	1.0%
Q42	1.0%
L48	1.0%
I49	1.0%
R50	1.0%
N51	1.0%
Y52	1.0%
V53	1.0%
A54	1.0%
R55	1.0%
P56	1.0%
T57	1.0%
A58	1.0%
C62	1.0%
R63	1.0%
N64	1.0%
R65	1.0%
T66	1.0%
R69	1.0%
R70	1.0%
R71	1.0%
Y74	1.0%
L75	1.0%
R76	1.0%
R77	1.0%
E78	1.0%
H82	1.0%
G83	1.0%
G84	1.0%
N89	1.0%
Q90	1.0%
Y91	1.0%
L92	1.0%
G93	1.0%
Q94	1.0%
A95	1.0%
L96	1.0%
L97	1.0%
R100	1.0%
M101	1.0%
G102	1.0%
K103	1.0%
S104	1.0%
E105	1.0%
I106	1.0%
E109	1.0%
A112	1.0%
G113	1.0%
Q114	1.0%
H115	1.0%
A118	1.0%
S119	1.0%
A120	1.0%
L121	1.0%
A122	1.0%
S123	1.0%
A124	1.0%
L125	1.0%
L126	1.0%
C130	1.0%
R131	1.0%
P132	1.0%
T133	1.0%
Y133	1.0%
M134	1.0%
D139	1.0%
R141	1.0%
Q142	1.0%
R143	1.0%
P144	1.0%
R145	1.0%
V146	1.0%
F147	1.0%
R148	1.0%
L149	1.0%
R150	1.0%
L151	1.0%
M152	1.0%
E155	1.0%
P158	1.0%
S163	1.0%
A164	1.0%
T165	1.0%
L166	1.0%
K167	1.0%
D168	1.0%
A169	1.0%
C170	1.0%
N171	1.0%
R175	1.0%
D176	1.0%
V177	1.0%
S178	1.0%
Y181	1.0%
M187	1.0%
L188	1.0%
G189	1.0%
T190	1.0%
A191	1.0%
H195	1.0%
P196	1.0%
R206	1.0%
M207	1.0%
Q215	1.0%
L216	1.0%
L217	1.0%
G221	1.0%
R222	1.0%
L223	1.0%
P224	1.0%
D225	1.0%
A226	1.0%
V227	1.0%
G234	1.0%
S235	1.0%
N236	1.0%
A237	1.0%
L238	1.0%
R239	1.0%
A242	1.0%
F241	1.0%
D243	1.0%
N245	1.0%
R241	1.0%
I345	1.0%
I346	1.0%
I347	1.0%
A348	1.0%
S351	1.0%
S352	1.0%
H353	1.0%
A356	1.0%
H357	1.0%
M362	1.0%
R363	1.0%
E364	1.0%
E367	1.0%
K368	1.0%
R379	1.0%
D383	1.0%
I384	1.0%
F385	1.0%
L386	1.0%
R387	1.0%
H388	1.0%
D389	1.0%
I390	1.0%
L391	1.0%
LYS	1.0%
ALA	1.0%
ARG	1.0%
GLY	1.0%
LEU	1.0%
ILE	1.0%

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.20Å 61.80Å 67.80Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	8.00 – 1.90 8.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	84.9 (8.00-1.90) 88.5 (8.00-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.86Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.186 , (Not available) 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 98.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5184	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: NA, PLP

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	0.89	0/1988	2.02	54/2698 (2.0%)
2	B	1.15	1/3043 (0.0%)	2.17	123/4112 (3.0%)
All	All	1.05	1/5031 (0.0%)	2.11	177/6810 (2.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	13	GLY	N-CA	5.77	1.51	1.45

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	ARG	CD-NE-CZ	12.11	141.36	124.40
2	B	34	ARG	CD-NE-CZ	12.11	141.35	124.40
1	A	233	SER	CA-C-N	11.46	132.87	120.03
1	A	233	SER	C-N-CA	11.46	132.87	120.03
2	B	234	GLY	N-CA-C	11.05	131.78	115.64
2	B	189	GLY	N-CA-C	10.74	126.49	114.67
2	B	390	ILE	N-CA-C	-10.45	102.82	111.81
2	B	175	ARG	CD-NE-CZ	10.41	138.97	124.40
2	B	206	ARG	CD-NE-CZ	9.83	138.16	124.40
1	A	204	HIS	CA-CB-CG	-9.81	103.99	113.80
1	A	140	ARG	CD-NE-CZ	-9.50	111.10	124.40
1	A	63	THR	O-C-N	9.18	131.52	122.07
2	B	273	HIS	CA-CB-CG	-9.16	104.64	113.80
2	B	119	SER	O-C-N	8.95	131.76	122.09
1	A	140	ARG	NE-CZ-NH1	-8.77	112.73	121.50
1	A	140	ARG	NE-CZ-NH2	8.72	127.05	119.20
1	A	234	GLY	CA-C-O	-8.41	112.56	120.80
2	B	100	ARG	CD-NE-CZ	-8.19	112.94	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	VAL	O-C-N	7.97	128.53	121.12
1	A	164	ARG	CD-NE-CZ	7.96	135.55	124.40
2	B	195	HIS	CA-CB-CG	7.76	121.56	113.80
2	B	100	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	A	168	SER	N-CA-C	7.57	120.60	111.82
1	A	104	ASN	CA-C-O	-7.49	112.62	120.55
1	A	63	THR	N-CA-CB	7.44	120.79	110.01
2	B	368	LYS	O-C-N	7.43	131.70	123.22
2	B	123	SER	O-C-N	7.42	130.10	122.09
2	B	125	LEU	N-CA-C	7.41	119.44	111.36
2	B	275	ARG	CA-C-O	-7.24	112.93	121.11
2	B	65[A]	ILE	CA-C-O	-7.16	110.92	119.58
2	B	65[B]	ILE	CA-C-O	-7.16	110.92	119.58
1	A	245	LEU	CA-C-N	7.14	129.72	120.44
1	A	245	LEU	C-N-CA	7.14	129.72	120.44
2	B	291	ASP	CA-CB-CG	7.13	119.73	112.60
2	B	275	ARG	CD-NE-CZ	-7.10	114.46	124.40
2	B	191	ALA	CA-C-N	7.08	133.94	122.53
2	B	191	ALA	C-N-CA	7.08	133.94	122.53
2	B	357	HIS	CA-CB-CG	-7.01	106.79	113.80
1	A	140	ARG	CA-CB-CG	6.88	127.87	114.10
2	B	215	GLN	OE1-CD-NE2	-6.88	115.72	122.60
2	B	226	ALA	CA-C-O	-6.87	113.30	120.99
2	B	241	PHE	N-CA-C	6.82	119.73	111.82
2	B	286	MET	O-C-N	6.79	130.90	123.10
2	B	308	SER	CA-C-N	6.72	131.31	122.51
2	B	308	SER	C-N-CA	6.72	131.31	122.51
2	B	341	ARG	CD-NE-CZ	6.68	133.76	124.40
2	B	30	GLU	CA-C-N	6.66	129.21	120.28
2	B	30	GLU	C-N-CA	6.66	129.21	120.28
1	A	55	SER	CA-C-O	-6.62	113.53	120.55
2	B	275	ARG	NE-CZ-NH1	-6.61	114.89	121.50
2	B	119	SER	CA-C-O	-6.60	113.91	120.70
2	B	250	VAL	CA-C-N	6.51	127.17	120.60
2	B	250	VAL	C-N-CA	6.51	127.17	120.60
2	B	241	PHE	CA-CB-CG	6.50	120.30	113.80
2	B	77	ARG	N-CA-C	6.42	119.25	109.62
2	B	190	THR	CA-CB-OG1	-6.36	100.06	109.60
2	B	235	SER	CA-C-O	-6.35	113.19	120.24
2	B	165	THR	N-CA-CB	-6.33	100.74	111.31
1	A	159	ASP	CA-CB-CG	6.31	118.91	112.60
2	B	167	LYS	CA-C-N	6.29	129.34	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	167	LYS	C-N-CA	6.29	129.34	120.28
1	A	136	SER	O-C-N	6.29	131.07	122.46
2	B	40	GLU	CA-CB-CG	6.26	126.63	114.10
2	B	286	MET	CA-C-O	-6.24	114.78	121.45
2	B	38	ASP	O-C-N	6.23	126.28	121.23
2	B	84	GLY	CA-C-O	-6.21	111.92	119.06
2	B	17	VAL	O-C-N	6.13	127.03	121.57
2	B	65[A]	ILE	O-C-N	6.11	130.55	122.12
2	B	65[B]	ILE	O-C-N	6.11	130.55	122.12
2	B	51	ASN	CA-CB-CG	-6.10	106.50	112.60
1	A	3	ARG	CA-C-O	-6.09	114.05	120.63
2	B	69	THR	N-CA-CB	-6.09	101.75	111.43
2	B	97	LEU	N-CA-C	-6.03	104.79	111.36
2	B	84	GLY	O-C-N	6.02	129.50	122.45
2	B	206	ARG	NE-CZ-NH1	6.02	127.52	121.50
2	B	30	GLU	CA-CB-CG	6.01	126.12	114.10
1	A	146	HIS	CA-CB-CG	-5.99	107.81	113.80
2	B	227	VAL	CB-CA-C	5.99	119.50	110.63
1	A	100	LEU	CB-CA-C	5.94	120.48	110.79
2	B	263	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	110	GLY	O-C-N	5.88	130.34	122.70
1	A	2	GLU	CB-CG-CD	5.87	122.59	112.60
2	B	256	GLU	O-C-N	5.86	128.30	121.21
2	B	314	ALA	N-CA-C	-5.83	104.92	111.28
2	B	188	LEU	CB-CA-C	5.82	119.60	109.65
2	B	132	ILE	O-C-N	5.81	129.48	123.20
2	B	58	ALA	O-C-N	5.81	129.47	122.85
2	B	383	ASP	CA-C-O	-5.76	112.59	119.15
2	B	334	GLU	CB-CG-CD	5.73	122.34	112.60
2	B	315	TYR	N-CA-C	5.71	117.31	111.14
1	A	31	GLU	CB-CG-CD	5.64	122.18	112.60
1	A	136	SER	CA-C-O	-5.64	112.67	119.27
2	B	227	VAL	N-CA-C	-5.63	100.22	108.11
2	B	78	GLU	N-CA-C	-5.62	106.38	113.18
2	B	243	ASP	CA-CB-CG	-5.62	106.98	112.60
2	B	167	LYS	CA-CB-CG	5.61	125.32	114.10
1	A	19	PHE	CA-CB-CG	-5.59	108.21	113.80
2	B	331	GLU	CG-CD-OE2	5.58	131.24	118.40
1	A	267	ARG	N-CA-C	-5.57	104.42	111.11
1	A	95	ILE	N-CA-C	5.57	114.41	108.95
2	B	35	ALA	CA-C-O	5.57	126.86	120.90
1	A	141	GLN	CA-CB-CG	-5.56	102.98	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	345	ILE	CA-C-N	-5.55	118.83	122.60
2	B	345	ILE	C-N-CA	-5.55	118.83	122.60
2	B	252	LEU	CA-C-O	-5.55	114.36	120.30
2	B	387	VAL	O-C-N	5.54	127.47	121.87
2	B	254	GLY	CA-C-O	-5.53	115.31	120.57
1	A	52	VAL	CA-C-O	-5.53	114.31	119.62
2	B	64	ASN	CA-C-O	-5.51	113.08	118.97
2	B	346	ILE	N-CA-C	-5.51	102.55	107.56
1	A	102	TYR	CA-C-O	-5.50	114.70	120.80
1	A	104	ASN	OD1-CG-ND2	5.50	128.10	122.60
2	B	323	ASP	CA-C-O	-5.49	114.89	120.71
2	B	106	ILE	CB-CG1-CD1	5.47	125.29	113.80
1	A	234	GLY	N-CA-C	5.46	119.49	112.83
2	B	18	PRO	CB-CA-C	5.45	118.37	111.39
2	B	12	PHE	CA-C-N	-5.43	117.03	122.63
2	B	12	PHE	C-N-CA	-5.43	117.03	122.63
2	B	69	THR	OG1-CB-CG2	5.42	120.13	109.30
1	A	216	SER	O-C-N	5.41	127.62	121.94
1	A	102	TYR	CA-CB-CG	-5.40	104.17	113.90
2	B	66	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	69	LEU	O-C-N	5.38	127.61	122.07
2	B	297	SER	CA-C-O	-5.38	114.46	120.54
1	A	232	ILE	CA-C-O	-5.38	114.82	120.57
1	A	49	GLU	CG-CD-OE1	-5.36	106.08	118.40
2	B	301	SER	CA-C-N	5.35	127.98	120.28
2	B	301	SER	C-N-CA	5.35	127.98	120.28
2	B	42	GLN	OE1-CD-NE2	-5.33	117.27	122.60
2	B	235	SER	N-CA-C	5.32	118.24	111.69
2	B	367	GLU	CB-CG-CD	5.31	121.62	112.60
1	A	141	GLN	CA-C-N	5.30	127.81	120.29
1	A	141	GLN	C-N-CA	5.30	127.81	120.29
2	B	95	ALA	CA-C-N	5.29	127.81	120.29
2	B	95	ALA	C-N-CA	5.29	127.81	120.29
2	B	362	MET	CA-C-O	-5.29	114.36	120.24
1	A	99	LEU	O-C-N	5.29	130.10	123.23
2	B	100	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	B	75	LEU	CA-C-O	-5.28	114.63	120.38
2	B	226	ALA	O-C-N	5.27	129.28	123.33
2	B	131	ARG	NE-CZ-NH1	5.26	126.76	121.50
2	B	236	ASN	CA-CB-CG	5.24	117.84	112.60
2	B	347	PRO	CB-CA-C	5.24	117.77	110.17
1	A	32	GLN	OE1-CD-NE2	-5.24	117.36	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	VAL	CB-CA-C	5.24	119.21	112.14
2	B	76	LYS	CB-CA-C	5.24	118.96	110.22
2	B	92	LEU	CA-C-O	-5.23	114.96	120.55
2	B	272	LYS	CA-C-O	-5.23	113.50	119.41
2	B	171	ASN	O-C-N	5.21	127.72	122.09
1	A	214	ILE	N-CA-CB	-5.19	105.08	111.00
1	A	155	PRO	CB-CA-C	5.19	117.25	110.92
2	B	338	THR	CA-CB-OG1	-5.18	101.83	109.60
2	B	282	MET	O-C-N	5.17	129.42	123.17
1	A	220	VAL	CB-CA-C	5.17	118.58	111.97
2	B	379	ARG	CA-CB-CG	5.16	124.43	114.10
1	A	130	ASP	N-CA-C	5.16	119.07	112.26
1	A	241	ILE	O-C-N	5.15	127.09	121.94
2	B	74	TYR	CA-C-O	-5.13	115.16	120.70
1	A	71	ALA	CA-C-N	5.13	127.10	120.44
1	A	71	ALA	C-N-CA	5.13	127.10	120.44
2	B	130	CYS	N-CA-CB	-5.12	101.95	110.80
2	B	168	ASP	CA-CB-CG	-5.12	107.48	112.60
2	B	267	HIS	O-C-N	5.11	129.33	122.73
2	B	222	ARG	CD-NE-CZ	5.11	131.56	124.40
2	B	151	LEU	O-C-N	5.10	127.52	122.12
2	B	341	ARG	CA-CB-CG	5.08	124.27	114.10
2	B	313	HIS	O-C-N	5.06	128.29	122.17
2	B	76	LYS	N-CA-C	-5.06	100.92	108.96
2	B	217	LEU	O-C-N	5.05	128.48	122.27
2	B	166	LEU	CA-C-N	5.05	127.36	120.54
2	B	166	LEU	C-N-CA	5.05	127.36	120.54
2	B	348	ALA	CA-C-N	5.03	127.72	120.38
2	B	348	ALA	C-N-CA	5.03	127.72	120.38
1	A	27	ASP	CA-C-O	-5.02	113.70	119.32
2	B	353	HIS	O-C-N	-5.02	116.67	122.09
1	A	80	GLN	O-C-N	5.01	129.15	122.43
2	B	308	SER	CA-C-O	-5.00	114.82	121.47

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	1945	0	1954	82	0
2	B	2962	0	2934	121	0
3	B	1	0	0	0	0
4	B	7	0	4	0	0
5	B	15	0	6	0	0
6	A	83	0	0	4	0
6	B	171	0	0	8	1
All	All	5184	0	4898	198	1

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 20.

All (198) 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:50:LYS:NZ	2:B:50:LYS:HB2	1.54	1.18
2:B:90:GLN:HE22	2:B:94:GLN:HE21	1.10	1.00
2:B:50:LYS:HB2	2:B:50:LYS:HZ2	1.05	0.99
1:A:63:THR:HG22	1:A:238:VAL:HG12	1.44	0.99
1:A:220:VAL:HG21	1:A:262:MET:HE3	1.44	0.97
2:B:6:ASN:HD22	2:B:8:TYR:H	1.13	0.96
2:B:6:ASN:ND2	2:B:8:TYR:H	1.64	0.96
2:B:271:LEU:HD12	2:B:271:LEU:O	1.68	0.92
1:A:22:PHE:HD2	1:A:49:GLU:HG2	1.33	0.91
2:B:31:ALA:HA	2:B:34:ARG:CD	2.03	0.89
2:B:65[B]:ILE:HD13	2:B:66:THR:HG23	1.55	0.88
2:B:50:LYS:NZ	2:B:50:LYS:CB	2.34	0.85
1:A:23:VAL:HG12	1:A:50:LEU:HD23	1.59	0.84
2:B:138:ASP:O	2:B:142:GLN:HB2	1.77	0.84
2:B:31:ALA:CB	2:B:101:MET:HE2	2.10	0.81
2:B:31:ALA:HB3	2:B:101:MET:HE2	1.63	0.81
2:B:69:THR:HG22	2:B:71:THR:H	1.43	0.81
2:B:34:ARG:HG2	2:B:100:ARG:HH21	1.45	0.81
2:B:31:ALA:HA	2:B:34:ARG:HD3	1.64	0.80
2:B:69:THR:CG2	2:B:71:THR:H	1.97	0.78
2:B:62:CYS:HB3	2:B:65[B]:ILE:HD11	1.66	0.77
1:A:220:VAL:CG2	1:A:262:MET:HE3	2.13	0.77
1:A:63:THR:HG22	1:A:238:VAL:CG1	2.16	0.75
2:B:50:LYS:HB2	2:B:50:LYS:HZ3	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLN:NE2	1:A:254:GLU:OE1	2.19	0.75
2:B:55:ARG:HH11	2:B:89:ASN:HD21	1.33	0.75
2:B:62:CYS:CB	2:B:65[B]:ILE:HD11	2.16	0.75
1:A:41:ILE:HD11	1:A:48:LEU:HD11	1.68	0.74
2:B:143:SER:HB2	2:B:144:PRO:HD3	1.68	0.74
1:A:194:HIS:O	1:A:198:GLU:HB2	1.87	0.74
1:A:31:GLU:H	1:A:31:GLU:CD	1.95	0.73
2:B:65[B]:ILE:CD1	2:B:66:THR:HG23	2.17	0.73
1:A:163:LEU:HD21	1:A:196:LEU:HD11	1.68	0.73
2:B:103:LYS:NZ	2:B:181:TYR:O	2.23	0.71
2:B:57:THR:OG1	2:B:76:LYS:HE3	1.90	0.71
1:A:22:PHE:CD2	1:A:49:GLU:HG2	2.24	0.70
1:A:63:THR:CG2	1:A:238:VAL:HG12	2.22	0.69
2:B:175:ARG:O	2:B:178:SER:HB2	1.94	0.68
2:B:29:GLU:OE2	2:B:195:HIS:HE1	1.76	0.68
2:B:31:ALA:HA	2:B:34:ARG:HD2	1.75	0.68
2:B:62:CYS:HB3	2:B:65[B]:ILE:CD1	2.24	0.68
2:B:142:GLN:O	2:B:146:VAL:HG23	1.94	0.67
2:B:133:TYR:OH	2:B:176:ASP:OD2	2.11	0.66
2:B:165:THR:CG2	6:B:442:HOH:O	2.42	0.66
1:A:23:VAL:HG12	1:A:50:LEU:CD2	2.26	0.66
2:B:34:ARG:CG	2:B:100:ARG:HH21	2.08	0.66
2:B:364:GLU:OE1	6:B:474:HOH:O	2.14	0.65
2:B:385:PHE:O	2:B:388:HIS:HB3	1.97	0.65
2:B:288:GLN:HE21	2:B:292:GLY:HA2	1.60	0.65
1:A:70:ARG:NH2	6:A:431:HOH:O	2.29	0.65
2:B:90:GLN:NE2	2:B:94:GLN:HE21	1.91	0.65
2:B:31:ALA:CB	2:B:34:ARG:HH11	2.10	0.64
1:A:178:SER:HB2	1:A:212:PHE:CB	2.27	0.64
1:A:199:LYS:HD2	1:A:203:TYR:CE2	2.33	0.64
1:A:156:PRO:HG3	1:A:179:ARG:H	1.63	0.63
1:A:220:VAL:CG2	1:A:262:MET:CE	2.76	0.63
1:A:154:CYS:HB3	1:A:176:LEU:HD12	1.79	0.63
2:B:386:THR:O	2:B:390:ILE:HG12	1.98	0.62
2:B:170:CYS:HB3	2:B:280:PHE:CE1	2.34	0.62
1:A:26:GLY:HA3	1:A:76:VAL:HG21	1.81	0.62
1:A:39:THR:HG23	1:A:256:ARG:HH11	1.67	0.60
2:B:165:THR:HG22	6:B:442:HOH:O	2.02	0.60
2:B:76:LYS:NZ	2:B:215:GLN:HE22	1.99	0.60
2:B:271:LEU:HD12	2:B:271:LEU:C	2.27	0.60
1:A:156:PRO:HG3	1:A:179:ARG:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ILE:HG21	2:B:224:PRO:HD3	1.83	0.59
2:B:95:ALA:HB2	2:B:187:MET:HE1	1.86	0.58
1:A:265:ALA:O	1:A:268:ALA:OXT	2.22	0.58
2:B:387:VAL:O	2:B:391:LEU:HG	2.04	0.58
2:B:6:ASN:HD22	2:B:6:ASN:C	2.12	0.58
1:A:14:ARG:O	1:A:15:ARG:C	2.47	0.57
2:B:333:LEU:O	2:B:337:LYS:HG3	2.03	0.57
1:A:70:ARG:HD3	1:A:245:LEU:HD21	1.85	0.57
1:A:22:PHE:HD2	1:A:49:GLU:CG	2.13	0.57
1:A:56:ASP:OD2	2:B:167:LYS:HG2	2.05	0.57
1:A:137:ALA:HB3	1:A:138:PRO:CD	2.35	0.56
2:B:28:LEU:HA	2:B:101:MET:HE1	1.87	0.56
2:B:66:THR:O	2:B:69:THR:HB	2.05	0.56
2:B:288:GLN:NE2	2:B:292:GLY:HA2	2.20	0.56
2:B:167:LYS:HB2	6:B:442:HOH:O	2.06	0.56
1:A:163:LEU:HD21	1:A:196:LEU:CD1	2.33	0.56
1:A:192:PRO:O	1:A:195:HIS:HB3	2.05	0.56
1:A:216:SER:N	1:A:219:GLN:OE1	2.38	0.56
1:A:117:ARG:O	1:A:117:ARG:HG3	2.07	0.55
2:B:272:LYS:HE3	6:B:410:HOH:O	2.06	0.54
2:B:69:THR:CG2	2:B:71:THR:HB	2.37	0.54
1:A:89:ARG:NH1	1:A:92:HIS:O	2.39	0.54
2:B:121:LEU:HB3	2:B:152:MET:CE	2.38	0.54
2:B:177:TRP:O	2:B:181:TYR:HB3	2.08	0.54
1:A:117:ARG:HD2	6:A:590:HOH:O	2.08	0.53
2:B:94:GLN:HB2	2:B:187:MET:HE2	1.91	0.53
1:A:104:ASN:HD21	2:B:288:GLN:NE2	2.07	0.53
2:B:334:GLU:HB2	6:B:515:HOH:O	2.08	0.53
2:B:69:THR:HG21	2:B:71:THR:HB	1.91	0.53
2:B:134:MET:O	2:B:158:PRO:HA	2.09	0.52
1:A:32:GLN:HB2	6:A:568:HOH:O	2.09	0.52
2:B:300:ILE:HB	2:B:329:ASP:CG	2.35	0.52
2:B:28:LEU:HD12	2:B:101:MET:HE1	1.92	0.51
2:B:76:LYS:HZ2	2:B:215:GLN:HE22	1.56	0.51
1:A:11:LEU:HD22	1:A:16:GLU:HG3	1.93	0.51
1:A:197:ILE:O	1:A:201:LYS:HG3	2.11	0.51
2:B:55:ARG:HD2	2:B:89:ASN:ND2	2.25	0.51
2:B:48:LEU:O	2:B:52:TYR:HB3	2.10	0.51
2:B:50:LYS:CB	2:B:50:LYS:HZ3	2.15	0.51
1:A:11:LEU:HD23	1:A:14:ARG:HH11	1.76	0.51
1:A:156:PRO:HG3	1:A:179:ARG:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:HIS:HD2	2:B:389:ASP:OD1	1.93	0.50
1:A:71:ALA:O	1:A:74:ALA:HB3	2.10	0.50
1:A:220:VAL:HG21	1:A:262:MET:CE	2.27	0.50
2:B:141:ARG:HG2	2:B:141:ARG:O	2.11	0.50
1:A:56:ASP:CG	2:B:167:LYS:HZ3	2.19	0.50
1:A:29:GLY:O	1:A:33:SER:HB2	2.11	0.50
2:B:146:VAL:O	2:B:150[A]:ARG:HG3	2.11	0.50
2:B:195:HIS:HD2	6:B:408:HOH:O	1.94	0.50
2:B:50:LYS:HZ2	2:B:50:LYS:CB	1.95	0.50
2:B:143:SER:N	2:B:144:PRO:CD	2.75	0.50
1:A:239:LYS:O	1:A:243:LYS:HG3	2.11	0.49
2:B:112:ALA:O	2:B:142:GLN:CG	2.60	0.49
1:A:258:PHE:O	1:A:262:MET:HG2	2.12	0.49
2:B:34:ARG:HG2	2:B:100:ARG:NH2	2.21	0.49
1:A:258:PHE:O	1:A:261:ALA:HB3	2.13	0.49
1:A:78:PRO:O	1:A:81:CYS:HB2	2.13	0.49
2:B:109:GLU:O	2:B:115:HIS:HD2	1.96	0.49
2:B:22:MET:N	2:B:23:PRO:CD	2.76	0.49
1:A:267:ARG:HG3	1:A:267:ARG:HH11	1.78	0.48
1:A:112:ASP:OD1	1:A:146:HIS:HE1	1.97	0.48
1:A:221:SER:OG	1:A:225:ARG:NH1	2.47	0.47
2:B:29:GLU:O	2:B:33:VAL:HG23	2.14	0.47
2:B:28:LEU:CD1	2:B:101:MET:HE1	2.44	0.47
1:A:250:GLN:NE2	1:A:250:GLN:O	2.47	0.47
2:B:171:ASN:O	2:B:175:ARG:HG3	2.14	0.47
1:A:22:PHE:C	1:A:22:PHE:CD1	2.93	0.47
2:B:28:LEU:HA	2:B:101:MET:CE	2.45	0.47
2:B:275:ARG:HH11	2:B:275:ARG:HD2	1.42	0.47
1:A:137:ALA:O	1:A:141:GLN:HG3	2.15	0.46
1:A:155:PRO:HD2	1:A:158:ALA:HB2	1.96	0.46
1:A:244:ASN:C	1:A:246:ALA:N	2.71	0.46
2:B:16:TYR:O	2:B:281:GLY:HA2	2.16	0.46
1:A:22:PHE:CE2	1:A:100:LEU:HD23	2.51	0.46
2:B:150[B]:ARG:HH21	2:B:155:GLU:HA	1.81	0.45
1:A:244:ASN:O	1:A:245:LEU:C	2.59	0.45
1:A:196:LEU:HD13	1:A:196:LEU:HA	1.69	0.45
2:B:91:VAL:HG11	2:B:118:ALA:O	2.16	0.45
2:B:115:HIS:CE1	2:B:189:GLY:HA2	2.52	0.45
2:B:26:ASN:O	2:B:30:GLU:HG3	2.16	0.45
2:B:163:SER:OG	2:B:168:ASP:OD2	2.30	0.44
1:A:216:SER:HA	1:A:217:PRO:HD3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:LEU:HD13	2:B:126:LEU:HD11	1.99	0.44
2:B:121:LEU:HB3	2:B:152:MET:HE1	1.99	0.44
2:B:287:MET:HE3	2:B:287:MET:HB3	1.86	0.44
2:B:69:THR:HG22	2:B:71:THR:N	2.23	0.44
1:A:107:PHE:O	1:A:108:ASN:C	2.61	0.44
1:A:267:ARG:HG3	1:A:267:ARG:NH1	2.32	0.44
2:B:53:ALA:HA	2:B:82:HIS:HB3	2.00	0.43
2:B:333:LEU:CD1	2:B:390:ILE:HG21	2.48	0.43
2:B:328:THR:OG1	2:B:331:GLU:HG3	2.18	0.43
1:A:104:ASN:HD21	2:B:288:GLN:HE22	1.65	0.43
2:B:246:ASN:HB2	6:B:544:HOH:O	2.18	0.43
1:A:37:ILE:O	1:A:41:ILE:HG13	2.18	0.43
2:B:31:ALA:HB2	2:B:34:ARG:HH11	1.80	0.43
2:B:55:ARG:NH1	2:B:89:ASN:HD21	2.07	0.43
1:A:89:ARG:HA	1:A:89:ARG:HD3	1.76	0.43
1:A:140:ARG:HH11	1:A:140:ARG:HD2	1.18	0.43
2:B:6:ASN:HD22	2:B:8:TYR:N	1.96	0.43
2:B:227:VAL:HG22	2:B:252:LEU:HD23	2.01	0.43
2:B:327:ILE:HG21	2:B:356:ALA:HB3	2.01	0.43
2:B:141:ARG:HH11	2:B:141:ARG:HD2	1.60	0.42
2:B:207:MET:HE3	2:B:207:MET:HB3	1.93	0.42
1:A:11:LEU:HD23	1:A:14:ARG:NH1	2.33	0.42
1:A:177:LEU:HG	1:A:178:SER:H	1.85	0.42
2:B:333:LEU:HD11	2:B:390:ILE:HG21	2.01	0.42
2:B:143:SER:CB	2:B:144:PRO:HD3	2.41	0.42
2:B:146:VAL:HA	2:B:149:MET:HE3	2.02	0.42
1:A:117:ARG:NH1	6:A:590:HOH:O	2.51	0.42
1:A:167:ALA:CB	1:A:205:ALA:HB2	2.50	0.42
2:B:217:LEU:O	2:B:221:GLY:HA2	2.19	0.42
1:A:56:ASP:OD2	2:B:167:LYS:NZ	2.47	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.84	0.41
1:A:21:PRO:HD2	1:A:47:ALA:O	2.20	0.41
1:A:195:HIS:O	1:A:198:GLU:HB3	2.20	0.41
2:B:6:ASN:ND2	2:B:8:TYR:N	2.48	0.41
2:B:298:TYR:CD2	2:B:298:TYR:C	2.98	0.41
1:A:112:ASP:OD2	1:A:145:ARG:NH2	2.38	0.41
1:A:137:ALA:HB3	1:A:138:PRO:HD3	2.02	0.41
1:A:213:GLY:O	1:A:219:GLN:NE2	2.54	0.41
2:B:90:GLN:HE22	2:B:94:GLN:NE2	1.94	0.41
2:B:125:LEU:O	2:B:125:LEU:HG	2.21	0.41
2:B:148:ARG:HE	2:B:148:ARG:HB2	1.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:SER:HA	2:B:238:ILE:HG22	2.03	0.41
1:A:57:PRO:C	1:A:59:ALA:H	2.28	0.41
2:B:256:GLU:O	2:B:326:SER:HA	2.21	0.41
2:B:333:LEU:HD23	2:B:333:LEU:HA	1.91	0.40
2:B:31:ALA:O	2:B:34:ARG:HD3	2.22	0.40
1:A:95:ILE:HA	1:A:96:PRO:HD3	1.81	0.40
1:A:130:ASP:OD1	1:A:130:ASP:N	2.55	0.40
2:B:31:ALA:CA	2:B:34:ARG:HD3	2.42	0.40
2:B:195:HIS:CD2	2:B:196:PRO:HA	2.57	0.40

All (1) 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)
6:B:488:HOH:O	6:B:488:HOH:O[2_655]	2.14	0.06

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	254/268 (95%)	239 (94%)	12 (5%)	3 (1%)	10	4
2	B	391/397 (98%)	381 (97%)	10 (3%)	0	100	100
All	All	645/665 (97%)	620 (96%)	22 (3%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	PHE
1	A	15	ARG
1	A	108	ASN

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	202/208 (97%)	177 (88%)	25 (12%)	4	1
2	B	309/311 (99%)	283 (92%)	26 (8%)	10	4
All	All	511/519 (98%)	460 (90%)	51 (10%)	8	3

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	10[A]	GLN
1	A	10[B]	GLN
1	A	14	ARG
1	A	23	VAL
1	A	31	GLU
1	A	35	LYS
1	A	49	GLU
1	A	80	GLN
1	A	112	ASP
1	A	120	GLN
1	A	121	VAL
1	A	123	VAL
1	A	127	LEU
1	A	133	VAL
1	A	140	ARG
1	A	164	ARG
1	A	193	LEU
1	A	194	HIS
1	A	196	LEU
1	A	197	ILE
1	A	210	GLN
1	A	215	SER
1	A	254	GLU
1	A	256	ARG
2	B	6	ASN
2	B	34	ARG

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Mol	Chain	Res	Type
2	B	40	GLU
2	B	50	LYS
2	B	65[A]	ILE
2	B	65[B]	ILE
2	B	69	THR
2	B	90	GLN
2	B	91	VAL
2	B	96	LEU
2	B	105	GLU
2	B	114	GLN
2	B	141	ARG
2	B	142	GLN
2	B	150[A]	ARG
2	B	150[B]	ARG
2	B	165	THR
2	B	188	LEU
2	B	216	ILE
2	B	222	ARG
2	B	271	LEU
2	B	276	VAL
2	B	283	LYS
2	B	296	GLU
2	B	297	SER
2	B	351	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	GLN
1	A	68	ASN
1	A	120	GLN
1	A	244	ASN
1	A	250	GLN
2	B	6	ASN
2	B	27	GLN
2	B	44	GLN
2	B	89	ASN
2	B	90	GLN
2	B	94	GLN
2	B	115	HIS
2	B	145	ASN
2	B	160	HIS

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Mol	Chain	Res	Type
2	B	195	HIS
2	B	215	GLN
2	B	288	GLN
2	B	317	ASN
2	B	370	GLN
2	B	388	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
5	PLP	B	401	4	15,15,16	1.91	6 (40%)	21,22,23	2.86	8 (38%)
4	SER	B	398	5	4,6,6	0.98	0	2,7,7	1.56	1 (50%)

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
5	PLP	B	401	4	-	0/6/6/8	0/1/1/1
4	SER	B	398	5	-	0/6/6/6	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	401	PLP	P-O4P	-3.75	1.48	1.60
5	B	401	PLP	C5-C4	-3.18	1.36	1.40
5	B	401	PLP	P-O1P	-2.80	1.41	1.50
5	B	401	PLP	P-O3P	-2.37	1.46	1.54
5	B	401	PLP	O3-C3	-2.35	1.31	1.36
5	B	401	PLP	P-O2P	2.13	1.62	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	401	PLP	O3P-P-O4P	9.25	130.79	106.67
5	B	401	PLP	O3-C3-C2	4.13	126.14	117.58
5	B	401	PLP	O4P-C5A-C5	4.00	116.85	109.36
5	B	401	PLP	C5-C6-N1	-3.25	118.55	123.83
5	B	401	PLP	C6-N1-C2	3.05	124.73	119.20
5	B	401	PLP	C4A-C4-C5	-2.70	118.15	120.94
5	B	401	PLP	C3-C2-N1	-2.48	117.83	120.96
4	B	398	SER	OXT-C-O	-2.20	119.09	124.08
5	B	401	PLP	C3-C4-C5	2.06	121.06	118.59

There are no chirality outliers.

There are no torsion outliers.

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 [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	257/268 (95%)	-0.30	3 (1%) 76 79	18, 38, 72, 102	1 (0%)
2	B	389/397 (97%)	-0.82	0 100 100	9, 23, 44, 70	4 (1%)
All	All	646/665 (97%)	-0.62	3 (0%) 87 89	9, 28, 60, 102	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	180	SER	3.9
1	A	193	LEU	2.3
1	A	194	HIS	2.2

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
4	SER	B	398	7/7	0.96	0.04	18,20,25,25	0
3	NA	B	400	1/1	0.98	0.04	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PLP	B	401	15/16	0.99	0.04	11,23,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.