



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:11 AM UTC

PDB ID : 1SPB / pdb_00001spb
Title : SUBTILISIN BPN' PROSEGMENT (77 RESIDUES) COMPLEXED WITH A MUTANT SUBTILISIN BPN' (266 RESIDUES). CRYSTAL PH 4.6. CRYSTALLIZATION TEMPERATURE 20 C DIFFRACTION TEMPERATURE-160 C
Authors : Gallagher, D.T.; Gilliland, G.L.; Wang, L.; Bryan, P.N.
Deposited on : 1995-06-21
Resolution : 2.00 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
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

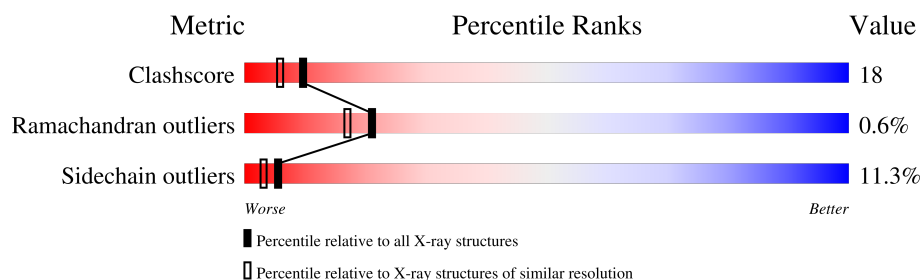
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	P	78	
2	S	266	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2668 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 SUBTILISIN BPN' PROSEGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	71	Total	C	N	O	S	0	0	0
			557	354	93	108	2			

- Molecule 2 is a protein called SUBTILISIN BPN'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	264	Total	C	N	O	S	0	0	0
			1860	1159	321	376	4			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	32	ASN	ASP	engineered mutation	UNP P00782
S	43	ASN	LYS	engineered mutation	UNP P00782
S	50	PHE	MET	engineered mutation	UNP P00782
S	73	LEU	ALA	engineered mutation	UNP P00782
S	?	-	LEU	deletion	UNP P00782
S	?	-	ASN	deletion	UNP P00782
S	?	-	ASN	deletion	UNP P00782
S	?	-	SER	deletion	UNP P00782
S	?	-	ILE	deletion	UNP P00782
S	?	-	GLY	deletion	UNP P00782
S	?	-	VAL	deletion	UNP P00782
S	?	-	LEU	deletion	UNP P00782
S	?	-	GLY	deletion	UNP P00782
S	206	VAL	GLN	engineered mutation	UNP P00782
S	217	LYS	TYR	engineered mutation	UNP P00782
S	218	SER	ASN	engineered mutation	UNP P00782
S	221	ALA	SER	engineered mutation	UNP P00782

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

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

- Molecule 4 is water.

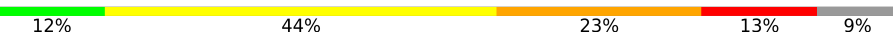
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	55	Total 55	O 55	0	0
4	S	195	Total 195	O 195	0	0

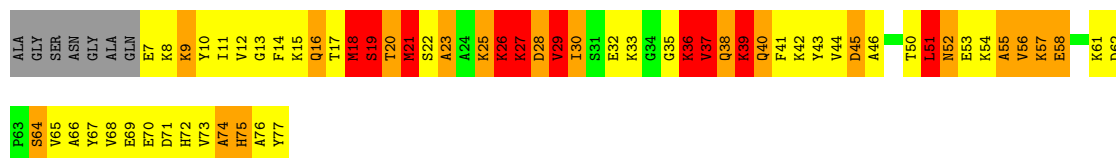
3 Residue-property plots

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.

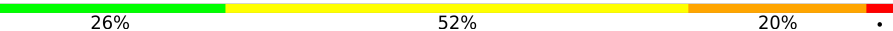
Note EDS was not executed.

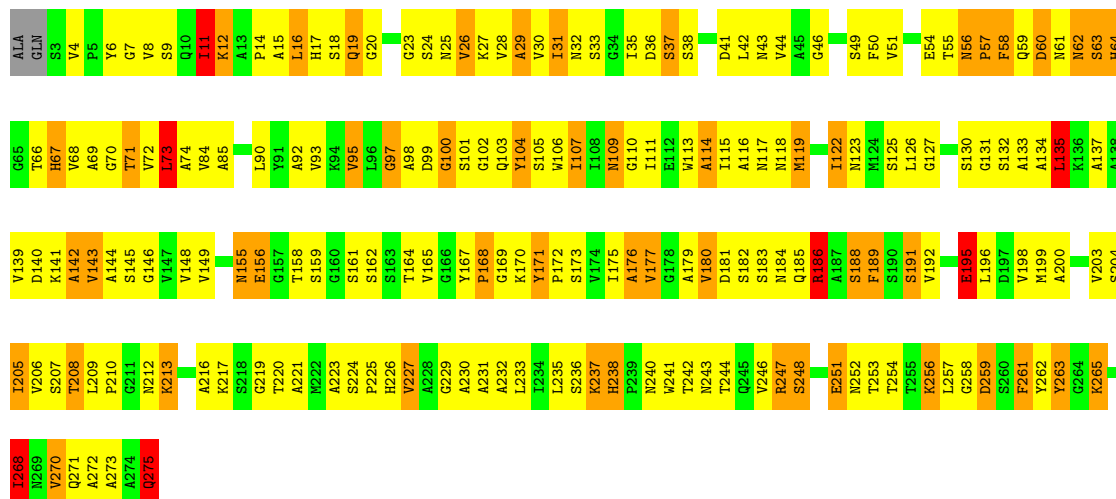
• Molecule 1: SUBTILISIN BPN' PROSEGMENT

Chain P: 



• Molecule 2: SUBTILISIN BPN'

Chain S: 



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	74.10Å 77.85Å 57.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2668	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

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

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	P	1.56	4/565 (0.7%)	3.37	95/752 (12.6%)
2	S	1.76	21/1898 (1.1%)	3.42	327/2592 (12.6%)
All	All	1.71	25/2463 (1.0%)	3.41	422/3344 (12.6%)

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	P	0	4
2	S	0	13
All	All	0	17

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	32	ASN	CA-CB	8.62	1.62	1.54
2	S	226	HIS	ND1-CE1	7.87	1.40	1.32
2	S	20	GLY	N-CA	-7.64	1.34	1.45
2	S	257	LEU	C-O	6.77	1.32	1.24
2	S	238	HIS	CA-CB	6.73	1.60	1.53
2	S	148	VAL	CA-C	6.72	1.60	1.52
2	S	42	LEU	N-CA	-6.61	1.38	1.46
2	S	51	VAL	N-CA	6.36	1.51	1.46
2	S	156	GLU	CA-C	-6.24	1.44	1.52
1	P	19	SER	CA-CB	6.08	1.63	1.53
2	S	85	ALA	CA-CB	5.91	1.60	1.53
2	S	219	GLY	N-CA	5.70	1.51	1.45
2	S	30	VAL	N-CA	5.61	1.52	1.46
2	S	268	ILE	CA-C	5.48	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	19	SER	C-O	5.46	1.30	1.24
2	S	203	VAL	N-CA	5.44	1.52	1.46
2	S	123	ASN	CA-C	5.38	1.59	1.52
2	S	27	LYS	CA-CB	-5.37	1.46	1.53
2	S	198	VAL	N-CA	5.28	1.51	1.46
2	S	200	ALA	C-O	5.27	1.28	1.24
2	S	273	ALA	C-O	5.25	1.30	1.24
2	S	146	GLY	C-O	5.23	1.30	1.24
1	P	67	TYR	N-CA	-5.09	1.39	1.46
1	P	50	THR	CB-OG1	5.06	1.51	1.43
2	S	242	THR	N-CA	5.02	1.52	1.45

All (422) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	19	GLN	CA-C-N	15.80	152.38	121.41
2	S	19	GLN	C-N-CA	15.80	152.38	121.41
2	S	54	GLU	CB-CG-CD	15.60	139.12	112.60
2	S	186	ARG	CD-NE-CZ	15.43	146.00	124.40
2	S	259	ASP	CA-CB-CG	15.19	127.79	112.60
1	P	19	SER	N-CA-C	14.00	140.62	110.80
2	S	140	ASP	CA-CB-CG	13.99	126.59	112.60
2	S	142	ALA	CA-C-N	13.39	137.06	120.72
2	S	142	ALA	C-N-CA	13.39	137.06	120.72
2	S	41	ASP	CA-CB-CG	13.23	125.83	112.60
1	P	41	PHE	CA-CB-CG	12.56	126.36	113.80
1	P	62	ASP	CA-CB-CG	12.52	125.12	112.60
2	S	36	ASP	CA-CB-CG	12.20	124.80	112.60
2	S	60	ASP	CA-CB-CG	11.96	124.56	112.60
2	S	58	PHE	CA-CB-CG	11.70	125.50	113.80
2	S	115	ILE	N-CA-CB	11.41	123.55	110.65
1	P	20	THR	CA-CB-CG2	11.26	129.64	110.50
2	S	25	ASN	CA-CB-CG	11.07	123.67	112.60
2	S	207	SER	CA-C-N	11.00	136.34	120.95
2	S	207	SER	C-N-CA	11.00	136.34	120.95
2	S	118	ASN	CA-CB-CG	10.87	123.47	112.60
2	S	74	ALA	CA-C-N	10.84	134.25	120.70
2	S	74	ALA	C-N-CA	10.84	134.25	120.70
2	S	105	SER	CA-C-N	10.68	134.59	120.28
2	S	105	SER	C-N-CA	10.68	134.59	120.28
1	P	7	GLU	CB-CG-CD	10.64	130.69	112.60
1	P	57	LYS	CA-CB-CG	10.49	135.08	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	164	THR	CA-C-N	10.46	136.04	120.77
2	S	164	THR	C-N-CA	10.46	136.04	120.77
2	S	251	GLU	CB-CG-CD	10.20	129.94	112.60
2	S	231	ALA	CA-C-N	10.18	133.92	120.28
2	S	231	ALA	C-N-CA	10.18	133.92	120.28
2	S	261	PHE	CA-CB-CG	10.12	123.92	113.80
1	P	42	LYS	CA-CB-CG	9.95	134.00	114.10
2	S	66	THR	CA-C-N	9.95	133.97	120.44
2	S	66	THR	C-N-CA	9.95	133.97	120.44
1	P	68	VAL	N-CA-CB	9.87	126.59	111.99
2	S	7	GLY	CA-C-N	9.86	132.99	120.56
2	S	7	GLY	C-N-CA	9.86	132.99	120.56
1	P	53	GLU	CB-CG-CD	9.79	129.24	112.60
2	S	180	VAL	CA-CB-CG2	9.68	126.86	110.40
2	S	17	HIS	CA-CB-CG	9.62	123.42	113.80
2	S	243	ASN	CA-CB-CG	9.60	122.20	112.60
2	S	156	GLU	CB-CG-CD	9.60	128.91	112.60
1	P	26	LYS	CA-C-N	9.55	133.85	120.29
1	P	26	LYS	C-N-CA	9.55	133.85	120.29
1	P	14	PHE	CA-CB-CG	9.43	123.23	113.80
1	P	39	LYS	CA-CB-CG	9.21	132.53	114.10
2	S	16	LEU	CA-C-N	9.21	132.63	120.28
2	S	16	LEU	C-N-CA	9.21	132.63	120.28
1	P	37	VAL	CA-CB-CG1	9.19	126.02	110.40
2	S	32	ASN	O-C-N	-9.17	116.23	123.11
1	P	71	ASP	CA-CB-CG	9.17	121.77	112.60
2	S	155	ASN	CA-CB-CG	9.12	121.72	112.60
1	P	39	LYS	CA-C-O	9.07	131.26	120.20
2	S	212	ASN	CA-CB-CG	9.03	121.63	112.60
1	P	58	GLU	CA-C-N	9.01	132.35	120.28
1	P	58	GLU	C-N-CA	9.01	132.35	120.28
2	S	109	ASN	CA-CB-CG	8.93	121.53	112.60
2	S	164	THR	O-C-N	-8.91	111.45	122.24
2	S	212	ASN	CB-CA-C	8.81	123.67	111.86
2	S	176	ALA	CA-C-O	8.79	130.28	120.43
2	S	177	VAL	CA-CB-CG2	8.74	125.26	110.40
2	S	195	GLU	CB-CG-CD	8.72	127.43	112.60
2	S	93	VAL	CB-CA-C	8.66	122.79	111.53
2	S	61	ASN	OD1-CG-ND2	8.62	131.22	122.60
2	S	114	ALA	CA-C-N	8.59	131.20	120.72
2	S	114	ALA	C-N-CA	8.59	131.20	120.72
2	S	61	ASN	CA-CB-CG	8.58	121.18	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	275	GLN	CA-CB-CG	8.56	131.21	114.10
2	S	56	ASN	CA-CB-CG	8.54	121.14	112.60
2	S	32	ASN	CA-C-O	8.50	126.31	120.19
2	S	141	LYS	CA-CB-CG	8.50	131.10	114.10
2	S	72	VAL	N-CA-CB	8.47	119.52	110.62
1	P	58	GLU	CA-CB-CG	8.46	131.01	114.10
2	S	257	LEU	CB-CA-C	8.45	127.24	110.42
1	P	53	GLU	CA-CB-CG	8.41	130.92	114.10
2	S	243	ASN	CA-C-N	8.41	131.37	120.44
2	S	243	ASN	C-N-CA	8.41	131.37	120.44
2	S	62	ASN	CA-C-N	8.35	137.48	121.54
2	S	62	ASN	C-N-CA	8.35	137.48	121.54
2	S	51	VAL	N-CA-C	-8.31	99.33	107.55
1	P	70	GLU	CB-CG-CD	8.28	126.67	112.60
2	S	46	GLY	CA-C-O	8.24	128.47	121.05
2	S	247	ARG	NE-CZ-NH2	-8.15	111.86	119.20
2	S	99	ASP	CA-CB-CG	8.15	120.75	112.60
2	S	23	GLY	CA-C-N	8.14	134.20	121.26
2	S	23	GLY	C-N-CA	8.14	134.20	121.26
2	S	111	ILE	CA-C-N	8.09	131.12	120.28
2	S	111	ILE	C-N-CA	8.09	131.12	120.28
2	S	181	ASP	CA-CB-CG	8.02	120.62	112.60
2	S	17	HIS	CA-C-N	7.91	131.52	120.29
2	S	17	HIS	C-N-CA	7.91	131.52	120.29
2	S	257	LEU	O-C-N	-7.89	112.09	122.59
2	S	56	ASN	CB-CA-C	7.89	117.98	110.17
2	S	72	VAL	O-C-N	7.87	130.46	121.96
2	S	68	VAL	CA-C-N	7.81	131.08	120.38
2	S	68	VAL	C-N-CA	7.81	131.08	120.38
1	P	46	ALA	CA-C-O	7.81	129.58	121.23
2	S	270	VAL	CA-C-N	7.79	130.57	120.44
2	S	270	VAL	C-N-CA	7.79	130.57	120.44
1	P	9	LYS	CA-C-O	7.78	129.15	120.43
2	S	41	ASP	CA-C-N	7.77	134.42	123.07
2	S	41	ASP	C-N-CA	7.77	134.42	123.07
2	S	135	LEU	CA-C-O	-7.77	112.31	120.55
1	P	29	VAL	CA-CB-CG2	7.72	123.52	110.40
2	S	25	ASN	OD1-CG-ND2	7.67	130.27	122.60
2	S	259	ASP	CB-CA-C	7.62	121.78	109.90
2	S	44	VAL	CB-CA-C	7.61	121.19	110.84
2	S	144	ALA	CA-C-O	7.60	128.69	120.10
2	S	55	THR	CA-CB-CG2	7.59	123.40	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	229	GLY	CA-C-N	7.57	130.43	120.28
2	S	229	GLY	C-N-CA	7.57	130.43	120.28
2	S	67	HIS	CA-C-N	7.57	130.09	120.56
2	S	67	HIS	C-N-CA	7.57	130.09	120.56
2	S	6	TYR	CA-C-N	7.55	129.64	120.13
2	S	6	TYR	C-N-CA	7.55	129.64	120.13
2	S	212	ASN	CA-C-O	7.54	130.47	121.65
2	S	66	THR	CA-CB-CG2	7.54	123.31	110.50
2	S	253	THR	CA-C-O	7.50	128.44	119.59
2	S	43	ASN	CB-CG-ND2	7.50	127.64	116.40
2	S	199	MET	CA-C-N	7.46	136.47	123.11
2	S	199	MET	C-N-CA	7.46	136.47	123.11
2	S	253	THR	CA-C-N	7.45	132.00	120.75
2	S	253	THR	C-N-CA	7.45	132.00	120.75
1	P	43	TYR	CA-CB-CG	7.44	127.30	113.90
2	S	54	GLU	CA-CB-CG	7.43	128.96	114.10
2	S	73	LEU	CB-CA-C	7.34	125.66	110.31
2	S	188	SER	N-CA-C	7.34	121.14	111.75
1	P	36	LYS	CA-C-N	7.31	131.36	120.69
1	P	36	LYS	C-N-CA	7.31	131.36	120.69
2	S	265	LYS	CA-C-N	7.29	135.70	121.41
2	S	265	LYS	C-N-CA	7.29	135.70	121.41
2	S	106	TRP	CA-CB-CG	7.28	127.43	113.60
2	S	43	ASN	CA-CB-CG	7.25	119.84	112.60
2	S	161	SER	CA-C-O	7.23	127.40	119.15
1	P	17	THR	CB-CA-C	7.21	122.99	110.01
2	S	104	TYR	CA-C-N	7.21	130.25	120.44
2	S	104	TYR	C-N-CA	7.21	130.25	120.44
2	S	184	ASN	CA-CB-CG	7.17	119.77	112.60
2	S	156	GLU	N-CA-C	7.16	122.19	113.17
2	S	117	ASN	CA-C-N	7.15	132.28	122.34
2	S	117	ASN	C-N-CA	7.15	132.28	122.34
2	S	185	GLN	CB-CG-CD	7.13	124.72	112.60
1	P	77	TYR	CA-CB-CG	7.13	126.73	113.90
1	P	11	ILE	N-CA-CB	7.11	120.89	111.64
2	S	189	PHE	CA-CB-CG	7.10	120.90	113.80
1	P	73	VAL	CB-CA-C	7.09	121.39	110.83
1	P	28	ASP	CA-C-O	-7.07	113.42	120.70
2	S	12	LYS	CA-C-O	7.05	129.03	120.57
2	S	58	PHE	CA-C-O	7.03	127.79	119.28
2	S	196	LEU	CB-CA-C	7.02	120.79	110.26
1	P	66	ALA	CA-C-N	7.01	135.08	121.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	66	ALA	C-N-CA	7.01	135.08	121.63
2	S	143	VAL	N-CA-CB	6.97	118.53	110.65
2	S	11	ILE	CA-C-N	6.97	132.77	122.74
2	S	11	ILE	C-N-CA	6.97	132.77	122.74
2	S	60	ASP	CB-CA-C	6.95	121.93	110.74
2	S	71	THR	CA-CB-CG2	6.94	122.29	110.50
2	S	203	VAL	CB-CA-C	6.94	120.89	110.63
2	S	27	LYS	CA-C-O	6.93	127.78	120.36
2	S	37	SER	CA-C-N	6.93	132.29	120.72
2	S	37	SER	C-N-CA	6.93	132.29	120.72
2	S	107	ILE	N-CA-CB	6.89	119.39	110.57
2	S	164	THR	CA-C-O	6.87	127.50	119.32
2	S	30	VAL	CB-CA-C	6.86	120.91	111.31
2	S	133	ALA	CA-C-N	6.82	129.72	120.44
2	S	133	ALA	C-N-CA	6.82	129.72	120.44
1	P	72	HIS	CA-CB-CG	6.81	120.61	113.80
1	P	45	ASP	CA-CB-CG	6.80	119.40	112.60
2	S	268	ILE	N-CA-CB	6.80	119.24	110.13
1	P	57	LYS	CB-CG-CD	6.77	126.86	111.30
2	S	247	ARG	NE-CZ-NH1	6.76	128.26	121.50
2	S	140	ASP	CA-C-N	6.75	129.88	120.29
2	S	140	ASP	C-N-CA	6.75	129.88	120.29
2	S	206	VAL	CA-C-O	6.75	128.55	120.65
2	S	254	THR	CA-CB-CG2	6.75	121.97	110.50
1	P	12	VAL	CB-CA-C	6.73	120.20	110.98
2	S	73	LEU	N-CA-CB	-6.72	99.23	110.39
2	S	104	TYR	CA-CB-CG	6.71	125.98	113.90
2	S	185	GLN	CA-CB-CG	6.71	127.52	114.10
1	P	51	LEU	CA-C-O	6.70	127.76	120.32
1	P	8	LYS	CA-CB-CG	6.69	127.48	114.10
2	S	179	ALA	CA-C-N	6.66	133.36	122.64
2	S	179	ALA	C-N-CA	6.66	133.36	122.64
1	P	19	SER	O-C-N	-6.64	113.76	122.59
2	S	205	ILE	CB-CA-C	6.63	118.84	111.08
2	S	51	VAL	CB-CA-C	6.61	118.84	111.04
2	S	100	GLY	CA-C-N	6.59	132.82	122.94
2	S	100	GLY	C-N-CA	6.59	132.82	122.94
2	S	247	ARG	CA-C-O	-6.56	113.93	120.82
1	P	39	LYS	CB-CG-CD	6.56	126.39	111.30
2	S	12	LYS	CB-CA-C	6.56	121.56	111.39
2	S	275	GLN	CB-CA-C	6.56	122.56	110.10
2	S	57	PRO	CA-C-N	6.55	134.24	122.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	57	PRO	C-N-CA	6.55	134.24	122.38
2	S	43	ASN	OD1-CG-ND2	-6.54	116.06	122.60
2	S	8	VAL	CA-CB-CG1	6.53	121.50	110.40
2	S	161	SER	O-C-N	-6.50	113.91	122.42
2	S	11	ILE	CA-C-O	6.47	127.46	119.43
2	S	258	GLY	CA-C-O	6.46	131.81	120.57
1	P	52	ASN	CA-CB-CG	6.45	119.05	112.60
1	P	74	ALA	CA-C-O	6.45	128.45	121.16
2	S	253	THR	O-C-N	-6.44	114.59	122.25
2	S	200	ALA	O-C-N	-6.42	117.60	121.71
2	S	241	TRP	CA-CB-CG	6.40	125.77	113.60
2	S	244	THR	N-CA-CB	6.38	119.27	110.01
2	S	213	LYS	CA-C-N	6.38	132.57	122.62
2	S	213	LYS	C-N-CA	6.38	132.57	122.62
2	S	252	ASN	CA-CB-CG	6.38	118.98	112.60
2	S	26	VAL	CA-C-O	6.37	127.01	120.39
2	S	242	THR	CA-CB-CG2	6.36	121.31	110.50
2	S	4	VAL	CA-CB-CG2	6.34	121.18	110.40
2	S	184	ASN	CA-C-O	6.33	127.88	119.59
2	S	235	LEU	N-CA-C	6.31	120.08	112.38
2	S	118	ASN	CA-C-O	6.31	129.03	121.65
1	P	75	HIS	O-C-N	-6.30	114.96	123.15
1	P	20	THR	CB-CA-C	6.29	121.80	109.35
2	S	271	GLN	CB-CG-CD	6.27	123.25	112.60
2	S	32	ASN	CB-CG-ND2	6.26	125.78	116.40
2	S	28	VAL	CA-CB-CG2	6.24	121.01	110.40
2	S	203	VAL	CA-CB-CG2	6.23	121.00	110.40
1	P	43	TYR	CA-C-N	6.23	130.25	121.66
1	P	43	TYR	C-N-CA	6.23	130.25	121.66
1	P	29	VAL	CA-C-O	-6.22	113.86	120.64
1	P	68	VAL	O-C-N	6.22	129.43	123.03
2	S	247	ARG	CD-NE-CZ	6.21	133.10	124.40
2	S	115	ILE	N-CA-C	-6.20	104.59	110.42
2	S	63	SER	N-CA-CB	6.20	120.96	110.49
2	S	95	VAL	CB-CA-C	6.18	116.70	110.65
2	S	110	GLY	CA-C-N	6.17	128.33	120.56
2	S	110	GLY	C-N-CA	6.17	128.33	120.56
2	S	179	ALA	CA-C-O	6.13	127.06	120.38
1	P	73	VAL	CA-CB-CG1	6.12	120.81	110.40
2	S	206	VAL	CB-CA-C	6.12	118.37	110.96
1	P	9	LYS	O-C-N	-6.12	116.10	123.13
2	S	240	ASN	CB-CA-C	6.12	120.29	109.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	51	LEU	CA-CB-CG	6.10	137.65	116.30
2	S	135	LEU	CB-CA-C	6.10	120.91	110.79
2	S	273	ALA	N-CA-C	6.08	117.90	111.28
1	P	46	ALA	O-C-N	-6.07	116.92	123.42
2	S	148	VAL	N-CA-CB	6.07	117.75	110.95
2	S	199	MET	CA-C-O	6.04	127.23	120.70
2	S	70	GLY	CA-C-O	-6.04	113.66	120.30
2	S	143	VAL	CA-C-O	-6.02	114.20	121.18
1	P	54	LYS	CA-CB-CG	6.00	126.09	114.10
2	S	63	SER	CA-C-N	5.97	128.60	120.54
2	S	63	SER	C-N-CA	5.97	128.60	120.54
2	S	205	ILE	CA-CB-CG1	5.97	120.55	110.40
2	S	31	ILE	N-CA-CB	5.96	118.75	111.60
2	S	148	VAL	N-CA-C	-5.95	99.73	108.54
2	S	64	HIS	N-CA-CB	5.93	118.78	109.94
2	S	165	VAL	N-CA-CB	5.91	117.28	110.49
2	S	4	VAL	CA-CB-CG1	5.90	120.43	110.40
2	S	226	HIS	CA-CB-CG	5.90	119.70	113.80
2	S	16	LEU	N-CA-CB	5.89	118.88	110.16
2	S	56	ASN	CA-C-N	5.88	125.56	119.56
2	S	56	ASN	C-N-CA	5.88	125.56	119.56
2	S	221	ALA	CA-C-N	5.86	130.60	120.58
2	S	221	ALA	C-N-CA	5.86	130.60	120.58
2	S	12	LYS	CA-C-N	5.84	128.29	120.58
2	S	12	LYS	C-N-CA	5.84	128.29	120.58
2	S	139	VAL	CA-C-N	5.83	128.10	120.28
2	S	139	VAL	C-N-CA	5.83	128.10	120.28
2	S	182	SER	N-CA-C	5.83	118.41	111.71
1	P	55	ALA	CA-C-N	5.82	128.00	120.56
1	P	55	ALA	C-N-CA	5.82	128.00	120.56
2	S	220	THR	CA-CB-CG2	5.81	120.38	110.50
2	S	272	ALA	CA-C-N	5.81	128.06	120.28
2	S	272	ALA	C-N-CA	5.81	128.06	120.28
2	S	118	ASN	CB-CA-C	5.81	119.64	111.86
1	P	56	VAL	CA-C-O	-5.79	114.62	121.05
2	S	171	TYR	CB-CA-C	5.78	118.49	109.42
2	S	164	THR	OG1-CB-CG2	5.77	120.83	109.30
1	P	30	ILE	CB-CA-C	5.75	119.53	111.94
2	S	188	SER	CA-CB-OG	-5.74	99.62	111.10
2	S	229	GLY	O-C-N	-5.73	116.63	122.19
2	S	102	GLY	CA-C-O	5.73	128.43	121.61
2	S	162	SER	CB-CA-C	5.73	120.00	109.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	56	VAL	CA-CB-CG1	5.73	120.14	110.40
1	P	38	GLN	CA-CB-CG	5.72	125.55	114.10
2	S	93	VAL	CA-CB-CG2	5.68	120.06	110.40
1	P	25	LYS	CA-C-N	5.68	128.16	120.38
1	P	25	LYS	C-N-CA	5.68	128.16	120.38
1	P	74	ALA	O-C-N	-5.67	116.01	123.16
2	S	84	VAL	CA-C-O	-5.67	115.22	121.29
1	P	19	SER	CB-CA-C	-5.67	99.14	110.42
2	S	84	VAL	CA-CB-CG1	5.67	120.04	110.40
2	S	125	SER	CA-C-O	5.65	131.36	121.53
2	S	11	ILE	O-C-N	-5.64	114.75	122.26
1	P	54	LYS	CA-C-N	5.64	127.83	120.28
1	P	54	LYS	C-N-CA	5.64	127.83	120.28
2	S	226	HIS	CA-C-N	5.62	129.97	121.65
2	S	226	HIS	C-N-CA	5.62	129.97	121.65
1	P	36	LYS	CA-C-O	5.62	128.33	120.52
2	S	261	PHE	CA-C-N	5.61	132.01	122.36
2	S	261	PHE	C-N-CA	5.61	132.01	122.36
2	S	38	SER	CA-C-O	5.61	126.28	119.38
2	S	85	ALA	O-C-N	-5.60	116.27	121.36
1	P	30	ILE	N-CA-CB	5.59	117.35	110.64
2	S	98	ALA	N-CA-C	5.59	118.90	111.75
2	S	12	LYS	O-C-N	-5.58	112.89	122.20
2	S	149	VAL	CB-CA-C	5.57	119.09	110.96
2	S	207	SER	O-C-N	-5.57	115.38	122.78
1	P	68	VAL	N-CA-C	-5.56	99.50	107.78
2	S	29	ALA	CA-C-O	5.56	126.31	120.36
2	S	18	SER	CA-C-N	5.55	129.99	120.72
2	S	18	SER	C-N-CA	5.55	129.99	120.72
2	S	227	VAL	CA-CB-CG2	5.52	119.79	110.40
2	S	64	HIS	N-CA-C	5.51	117.73	111.11
2	S	223	ALA	O-C-N	-5.49	115.89	122.15
1	P	27	LYS	N-CA-CB	-5.49	102.04	110.16
2	S	224	SER	CA-C-N	5.48	125.82	119.47
2	S	224	SER	C-N-CA	5.48	125.82	119.47
1	P	77	TYR	CB-CA-C	5.48	120.50	110.10
2	S	42	LEU	N-CA-CB	5.47	119.30	110.65
2	S	117	ASN	CB-CA-C	5.47	119.85	110.01
2	S	16	LEU	CA-CB-CG	5.46	135.42	116.30
1	P	7	GLU	CA-CB-CG	5.45	125.00	114.10
2	S	117	ASN	CA-C-O	5.45	125.87	119.28
2	S	246	VAL	CB-CA-C	5.44	119.14	112.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	183	SER	O-C-N	-5.43	115.42	122.37
2	S	49	SER	CA-C-N	5.42	130.72	122.37
2	S	49	SER	C-N-CA	5.42	130.72	122.37
2	S	85	ALA	CA-C-O	5.42	128.06	120.64
1	P	64	SER	CA-C-N	5.41	129.90	123.19
1	P	64	SER	C-N-CA	5.41	129.90	123.19
2	S	195	GLU	CA-CB-CG	5.41	124.92	114.10
2	S	252	ASN	OD1-CG-ND2	-5.41	117.19	122.60
2	S	206	VAL	N-CA-CB	5.40	117.16	111.00
2	S	58	PHE	CA-C-N	5.40	130.61	123.05
2	S	58	PHE	C-N-CA	5.40	130.61	123.05
2	S	263	TYR	CA-C-O	5.39	124.89	118.69
2	S	168	PRO	N-CA-C	5.38	126.08	112.10
2	S	38	SER	O-C-N	-5.38	115.22	122.43
2	S	199	MET	O-C-N	-5.37	116.25	123.23
2	S	118	ASN	CA-C-N	5.37	128.47	120.95
2	S	118	ASN	C-N-CA	5.37	128.47	120.95
2	S	97	GLY	CA-C-N	5.36	128.20	120.38
2	S	97	GLY	C-N-CA	5.36	128.20	120.38
2	S	183	SER	CA-C-O	5.36	126.18	119.59
1	P	14	PHE	CB-CA-C	5.35	118.66	109.51
2	S	259	ASP	N-CA-CB	-5.34	101.52	109.69
2	S	159	SER	O-C-N	-5.34	115.34	122.28
1	P	57	LYS	N-CA-CB	5.34	118.06	110.16
2	S	144	ALA	N-CA-C	5.33	117.84	111.71
2	S	51	VAL	O-C-N	5.33	124.73	121.37
2	S	145	SER	N-CA-CB	-5.33	101.46	110.41
1	P	18	MET	CA-C-N	5.32	131.71	121.54
1	P	18	MET	C-N-CA	5.32	131.71	121.54
2	S	213	LYS	CG-CD-CE	5.31	123.52	111.30
2	S	38	SER	N-CA-C	5.31	119.01	112.54
2	S	122	ILE	CB-CG1-CD1	5.30	124.92	113.80
1	P	38	GLN	CB-CG-CD	5.29	121.60	112.60
2	S	235	LEU	CA-C-N	5.29	129.63	120.58
2	S	235	LEU	C-N-CA	5.29	129.63	120.58
2	S	270	VAL	CB-CA-C	5.29	119.52	112.22
1	P	14	PHE	CA-C-O	5.28	127.70	121.36
1	P	40	GLN	CA-C-N	5.28	128.20	120.71
1	P	40	GLN	C-N-CA	5.28	128.20	120.71
2	S	155	ASN	CB-CA-C	5.28	120.20	111.23
2	S	208	THR	CA-CB-CG2	5.28	119.47	110.50
2	S	115	ILE	CA-C-N	5.27	127.60	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	115	ILE	C-N-CA	5.27	127.60	120.38
2	S	115	ILE	CA-CB-CG1	5.26	119.35	110.40
1	P	45	ASP	CB-CA-C	5.26	119.91	111.91
2	S	33	SER	N-CA-CB	-5.24	102.87	110.47
2	S	145	SER	CA-C-N	5.22	129.45	121.51
2	S	145	SER	C-N-CA	5.22	129.45	121.51
2	S	130	SER	CA-C-O	5.22	126.59	120.80
1	P	73	VAL	CA-C-O	5.22	126.01	120.48
2	S	95	VAL	CA-C-N	5.22	130.49	122.93
2	S	95	VAL	C-N-CA	5.22	130.49	122.93
2	S	191	SER	N-CA-CB	5.21	117.70	109.83
2	S	107	ILE	CA-C-O	-5.21	115.27	121.05
2	S	233	LEU	CA-CB-CG	5.21	134.53	116.30
2	S	104	TYR	CB-CG-CD1	5.21	128.61	120.80
2	S	131	GLY	CA-C-N	5.21	130.10	122.39
2	S	131	GLY	C-N-CA	5.21	130.10	122.39
2	S	204	SER	CB-CA-C	5.21	119.28	111.89
2	S	204	SER	CA-C-O	5.20	127.88	121.84
2	S	144	ALA	O-C-N	-5.20	116.14	122.22
2	S	252	ASN	N-CA-C	5.19	119.33	112.89
2	S	179	ALA	N-CA-C	5.19	117.42	109.07
2	S	236	SER	CA-C-N	5.18	129.49	120.68
2	S	236	SER	C-N-CA	5.18	129.49	120.68
2	S	116	ALA	N-CA-C	5.18	117.60	111.33
1	P	13	GLY	O-C-N	-5.18	119.52	123.35
2	S	27	LYS	CA-CB-CG	5.18	124.45	114.10
2	S	85	ALA	CA-C-N	5.18	124.97	119.28
2	S	85	ALA	C-N-CA	5.18	124.97	119.28
2	S	253	THR	CA-CB-CG2	5.17	119.29	110.50
2	S	270	VAL	N-CA-C	5.16	115.93	110.72
1	P	21	MET	N-CA-CB	5.16	119.20	110.49
2	S	50	PHE	CB-CA-C	5.15	119.50	110.64
2	S	258	GLY	CA-C-N	5.15	128.08	120.82
2	S	258	GLY	C-N-CA	5.15	128.08	120.82
1	P	39	LYS	CA-C-N	5.15	129.26	122.42
1	P	39	LYS	C-N-CA	5.15	129.26	122.42
2	S	141	LYS	CB-CG-CD	5.15	123.14	111.30
1	P	29	VAL	N-CA-CB	5.14	118.61	110.54
2	S	59	GLN	CB-CA-C	5.13	118.60	110.19
1	P	53	GLU	CA-C-N	5.12	127.40	120.44
1	P	53	GLU	C-N-CA	5.12	127.40	120.44
2	S	107	ILE	CA-C-N	5.11	127.19	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	107	ILE	C-N-CA	5.11	127.19	120.60
2	S	51	VAL	CA-CB-CG2	5.11	119.08	110.40
2	S	220	THR	CA-C-O	5.11	125.67	119.49
2	S	84	VAL	N-CA-C	-5.10	105.35	110.30
2	S	263	TYR	O-C-N	-5.10	116.94	122.19
2	S	56	ASN	OD1-CG-ND2	-5.10	117.50	122.60
2	S	68	VAL	O-C-N	5.09	126.90	121.91
1	P	68	VAL	CA-CB-CG2	5.07	119.02	110.40
2	S	113	TRP	O-C-N	5.07	127.49	122.12
1	P	69	GLU	CB-CG-CD	5.06	121.20	112.60
2	S	204	SER	N-CA-C	5.05	118.36	111.39
2	S	113	TRP	CA-C-O	-5.05	115.20	120.55
2	S	227	VAL	N-CA-C	-5.03	106.77	111.45
1	P	43	TYR	CA-C-O	5.01	125.61	119.64
2	S	220	THR	OG1-CB-CG2	5.01	119.32	109.30
2	S	206	VAL	CA-CB-CG1	5.00	118.90	110.40
2	S	246	VAL	CA-CB-CG1	5.00	118.90	110.40

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	23	ALA	Mainchain
1	P	26	LYS	Mainchain
1	P	29	VAL	Mainchain
1	P	55	ALA	Mainchain
2	S	119	MET	Mainchain
2	S	126	LEU	Mainchain
2	S	134	ALA	Mainchain
2	S	135	LEU	Mainchain
2	S	142	ALA	Mainchain
2	S	191	SER	Mainchain
2	S	192	VAL	Mainchain
2	S	210	PRO	Mainchain
2	S	230	ALA	Mainchain
2	S	24	SER	Mainchain
2	S	248	SER	Mainchain
2	S	256	LYS	Mainchain
2	S	268	ILE	Mainchain

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	P	557	0	572	35	0
2	S	1860	0	1822	57	0
3	S	1	0	0	0	0
4	P	55	0	0	3	0
4	S	195	0	0	12	0
All	All	2668	0	2394	85	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 18.

All (85) 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:P:19:SER:CB	1:P:64:SER:HA	1.97	0.94
1:P:27:LYS:HG2	1:P:37:VAL:HG11	1.53	0.89
1:P:15:LYS:HD3	1:P:18:MET:HB3	1.55	0.85
2:S:35:ILE:HD12	2:S:92:ALA:HB2	1.59	0.85
1:P:36:LYS:HD3	1:P:38:GLN:HE22	1.48	0.79
2:S:12:LYS:HB3	4:S:536:HOH:O	1.84	0.77
2:S:256:LYS:HD2	4:S:396:HOH:O	1.83	0.77
1:P:19:SER:HB3	1:P:64:SER:HA	1.65	0.77
1:P:15:LYS:HB2	1:P:19:SER:HB2	1.66	0.76
2:S:31:ILE:HD12	2:S:122:ILE:HG23	1.70	0.71
1:P:15:LYS:CD	1:P:18:MET:HB3	2.19	0.71
1:P:9:LYS:HD3	2:S:103:GLN:NE2	2.10	0.67
1:P:74:ALA:HB3	2:S:107:ILE:HD11	1.76	0.67
2:S:26:VAL:HG11	2:S:232:ALA:HA	1.75	0.66
2:S:15:ALA:HB3	4:S:536:HOH:O	1.95	0.66
1:P:25:LYS:O	1:P:29:VAL:HG23	1.98	0.64
2:S:69:ALA:HB1	2:S:90:LEU:HD21	1.81	0.62
2:S:213:LYS:HE2	4:S:518:HOH:O	2.01	0.61
1:P:21:MET:HG3	4:P:534:HOH:O	2.03	0.58
1:P:27:LYS:HG2	1:P:37:VAL:CG1	2.31	0.58
2:S:104:TYR:HA	2:S:107:ILE:HD12	1.84	0.57
1:P:33:LYS:HD2	1:P:58:GLU:HB3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:14:PRO:HD2	4:S:512:HOH:O	2.04	0.57
1:P:15:LYS:HD3	1:P:18:MET:SD	2.45	0.57
1:P:10:TYR:CZ	1:P:56:VAL:HG21	2.40	0.56
2:S:158:THR:HG21	2:S:262:TYR:OH	2.05	0.56
2:S:132:SER:HB3	2:S:135:LEU:HB3	1.88	0.55
1:P:15:LYS:HD3	1:P:18:MET:CB	2.33	0.54
1:P:75:HIS:HA	2:S:100:GLY:O	2.08	0.54
1:P:9:LYS:HD3	2:S:103:GLN:CD	2.34	0.53
2:S:35:ILE:HD12	2:S:92:ALA:CB	2.37	0.53
1:P:16:GLN:HB2	1:P:21:MET:SD	2.49	0.53
2:S:31:ILE:HG22	2:S:95:VAL:HG21	1.91	0.53
2:S:35:ILE:O	2:S:58:PHE:HA	2.09	0.52
2:S:73:LEU:HD22	2:S:90:LEU:HD22	1.89	0.52
2:S:237:LYS:NZ	2:S:275:GLN:O	2.41	0.52
2:S:205:ILE:O	2:S:216:ALA:HA	2.09	0.52
2:S:31:ILE:HD12	2:S:122:ILE:CG2	2.39	0.52
1:P:23:ALA:O	1:P:27:LYS:HB2	2.09	0.51
2:S:169:GLY:O	2:S:176:ALA:HB2	2.09	0.51
1:P:19:SER:HB3	1:P:64:SER:CA	2.39	0.51
1:P:76:ALA:HB1	4:S:361:HOH:O	2.11	0.51
2:S:175:ILE:HG12	2:S:247:ARG:HG3	1.92	0.51
2:S:265:LYS:HE2	4:S:444:HOH:O	2.11	0.50
2:S:175:ILE:CG1	2:S:247:ARG:HG3	2.42	0.50
1:P:44:VAL:HG13	2:S:137:ALA:HB3	1.93	0.50
1:P:23:ALA:HA	1:P:40:GLN:OE1	2.13	0.48
1:P:74:ALA:O	2:S:101:SER:HA	2.14	0.48
2:S:143:VAL:HG21	2:S:173:SER:HB2	1.94	0.48
2:S:67:HIS:CE1	2:S:217:LYS:HB2	2.48	0.48
2:S:186:ARG:HB2	2:S:263:TYR:CZ	2.49	0.48
2:S:114:ALA:HB3	2:S:122:ILE:HD11	1.96	0.47
1:P:19:SER:HB3	1:P:64:SER:CB	2.45	0.47
2:S:251:GLU:HB3	2:S:265:LYS:HG3	1.97	0.47
2:S:31:ILE:HG22	2:S:95:VAL:CG2	2.45	0.47
2:S:37:SER:HB3	2:S:58:PHE:HB3	1.97	0.46
2:S:62:ASN:OD1	2:S:64:HIS:HD2	1.99	0.46
2:S:155:ASN:HA	2:S:189:PHE:O	2.16	0.45
1:P:10:TYR:HB2	1:P:51:LEU:HD22	1.98	0.45
2:S:97:GLY:HA3	4:S:439:HOH:O	2.17	0.44
2:S:67:HIS:HA	2:S:208:THR:O	2.17	0.44
2:S:29:ALA:HB2	2:S:119:MET:HG3	1.98	0.44
2:S:127:GLY:HA2	2:S:167:TYR:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:9:SER:HB3	4:S:367:HOH:O	2.18	0.43
2:S:56:ASN:HA	2:S:57:PRO:HD2	1.64	0.43
2:S:170:LYS:HG2	2:S:195:GLU:HG2	2.00	0.43
2:S:171:TYR:HA	2:S:172:PRO:HD3	1.90	0.43
2:S:114:ALA:CB	2:S:122:ILE:HD11	2.49	0.43
2:S:172:PRO:HD2	4:S:329:HOH:O	2.18	0.43
1:P:33:LYS:CD	1:P:58:GLU:HB3	2.47	0.43
1:P:39:LYS:HG2	2:S:109:ASN:HD21	1.84	0.43
2:S:177:VAL:HG11	2:S:227:VAL:CG2	2.48	0.43
1:P:15:LYS:HE3	1:P:65:VAL:O	2.18	0.42
1:P:52:ASN:ND2	4:P:445:HOH:O	2.51	0.42
2:S:261:PHE:HD2	4:S:513:HOH:O	2.02	0.42
2:S:209:LEU:HD21	2:S:217:LYS:HE2	2.02	0.42
2:S:256:LYS:HG3	4:S:396:HOH:O	2.19	0.42
1:P:30:ILE:HG23	1:P:35:GLY:HA3	2.02	0.41
4:P:326:HOH:O	2:S:64:HIS:HE1	2.03	0.41
2:S:11:ILE:O	2:S:270:VAL:HG12	2.20	0.41
2:S:71:THR:HG21	2:S:225:PRO:HG2	2.02	0.41
1:P:26:LYS:HE2	1:P:45:ASP:OD1	2.21	0.41
1:P:28:ASP:O	1:P:32:GLU:HG2	2.21	0.41
2:S:237:LYS:HD3	2:S:238:HIS:NE2	2.36	0.41
1:P:15:LYS:HB3	1:P:18:MET:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	69/78 (88%)	64 (93%)	4 (6%)	1 (1%)	9	4
2	S	262/266 (98%)	250 (95%)	11 (4%)	1 (0%)	30	27
All	All	331/344 (96%)	314 (95%)	15 (4%)	2 (1%)	21	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	63	SER
1	P	19	SER

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	P	59/62 (95%)	46 (78%)	13 (22%)	1	0
2	S	197/198 (100%)	181 (92%)	16 (8%)	11	7
All	All	256/260 (98%)	227 (89%)	29 (11%)	5	3

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	16	GLN
1	P	18	MET
1	P	20	THR
1	P	21	MET
1	P	22	SER
1	P	27	LYS
1	P	29	VAL
1	P	36	LYS
1	P	37	VAL
1	P	39	LYS
1	P	51	LEU
1	P	57	LYS
1	P	61	LYS
2	S	11	ILE
2	S	16	LEU
2	S	19	GLN
2	S	60	ASP
2	S	73	LEU
2	S	156	GLU
2	S	168	PRO
2	S	180	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	S	186	ARG
2	S	188	SER
2	S	195	GLU
2	S	237	LYS
2	S	248	SER
2	S	259	ASP
2	S	268	ILE
2	S	275	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	16	GLN
1	P	38	GLN
1	P	72	HIS
2	S	64	HIS
2	S	109	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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.