Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 08:54 AM EDT

PDB ID	:	1SPB
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

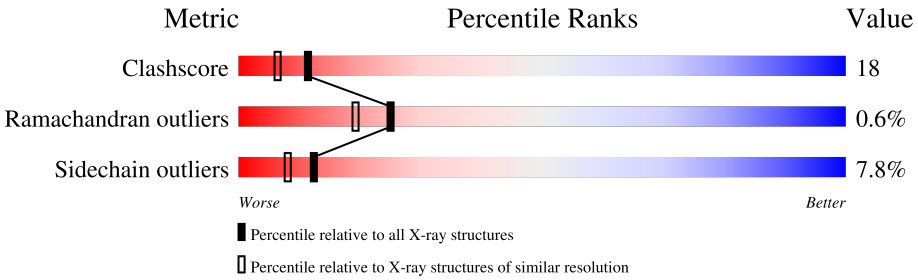
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	P	78	22% 47% 17% 5% 9%
2	S	266	45% 41% 12% ..

2 Entry composition (i)

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 (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

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

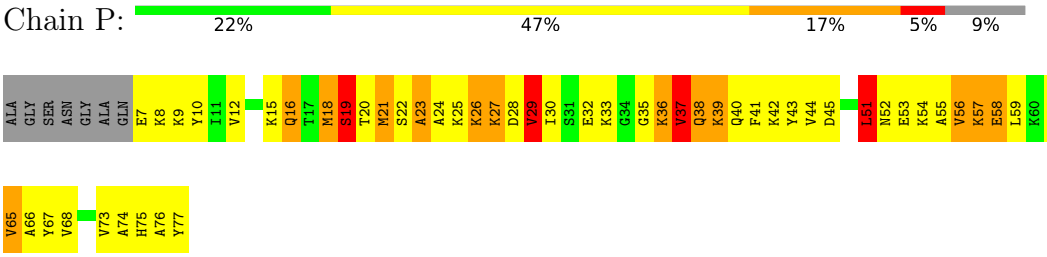
3 Residue-property plots (i)

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.

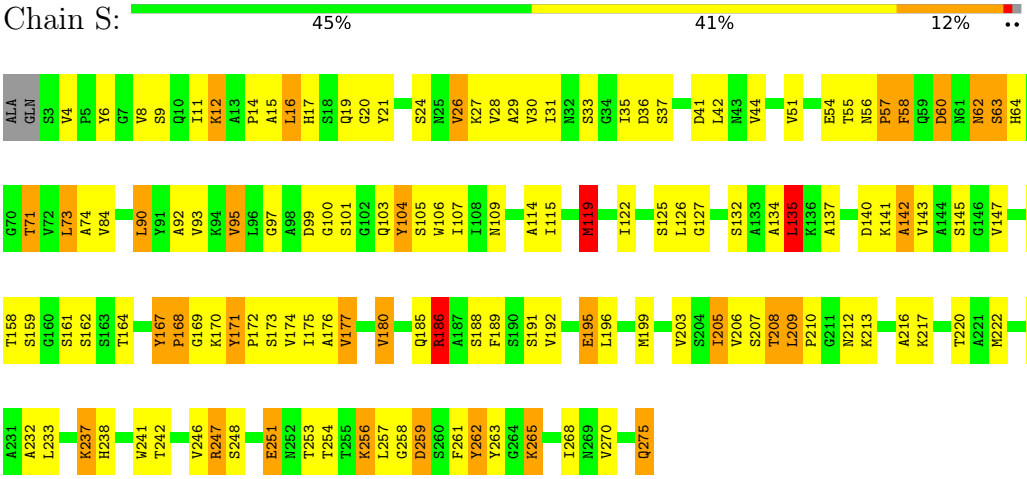
• Molecule 1: SUBTILISIN BPN' PROSEGMENT

Chain P:



• Molecule 2: SUBTILISIN BPN'

Chain S:



4 Data and refinement statistics (i)

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

5.1 Standard geometry

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	1.29	1/565 (0.2%)	2.59	45/752 (6.0%)
2	S	1.35	4/1898 (0.2%)	2.53	123/2592 (4.7%)
All	All	1.34	5/2463 (0.2%)	2.54	168/3344 (5.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	20	GLY	N-CA	-7.84	1.34	1.46
1	P	19	SER	CA-CB	7.19	1.63	1.52
2	S	54	GLU	CB-CG	-5.46	1.41	1.52
2	S	251	GLU	CG-CD	-5.25	1.44	1.51
2	S	54	GLU	CG-CD	-5.12	1.44	1.51

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	247	ARG	NE-CZ-NH2	-16.88	111.86	120.30
2	S	186	ARG	CD-NE-CZ	16.00	146.00	123.60
2	S	247	ARG	NE-CZ-NH1	15.92	128.26	120.30
2	S	19	GLN	C-N-CA	14.33	152.38	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	104	TYR	CB-CG-CD1	12.68	128.61	121.00
1	P	20	THR	CA-CB-CG2	12.31	129.64	112.40
2	S	171	TYR	CB-CG-CD1	11.59	127.95	121.00
1	P	19	SER	N-CA-C	10.97	140.62	111.00
2	S	171	TYR	CB-CG-CD2	-10.87	114.48	121.00
2	S	180	VAL	CA-CB-CG2	10.64	126.86	110.90
2	S	259	ASP	CB-CG-OD1	10.60	127.84	118.30
2	S	262	TYR	CB-CG-CD1	10.35	127.21	121.00
1	P	37	VAL	CA-CB-CG1	10.08	126.02	110.90
1	P	57	LYS	CA-CB-CG	9.85	135.08	113.40
1	P	51	LEU	CA-CB-CG	9.72	137.65	115.30
2	S	177	VAL	CA-CB-CG2	9.57	125.26	110.90
1	P	42	LYS	CA-CB-CG	9.37	134.00	113.40
2	S	262	TYR	CB-CG-CD2	-9.27	115.44	121.00
2	S	54	GLU	CB-CG-CD	9.23	139.12	114.20
2	S	41	ASP	CB-CG-OD1	9.13	126.52	118.30
2	S	257	LEU	CB-CA-C	8.97	127.24	110.20
2	S	140	ASP	CB-CG-OD1	8.92	126.33	118.30
2	S	16	LEU	CA-CB-CG	8.75	135.42	115.30
1	P	39	LYS	CA-CB-CG	8.69	132.53	113.40
2	S	104	TYR	CB-CG-CD2	-8.67	115.80	121.00
1	P	41	PHE	CB-CG-CD1	8.67	126.87	120.80
1	P	29	VAL	CA-CB-CG2	8.41	123.52	110.90
2	S	233	LEU	CA-CB-CG	8.36	134.53	115.30
2	S	259	ASP	CB-CG-OD2	-8.21	110.91	118.30
2	S	73	LEU	CB-CA-C	8.13	125.66	110.20
2	S	140	ASP	CB-CG-OD2	-8.11	111.00	118.30
2	S	275	GLN	CA-CB-CG	8.10	131.21	113.40
2	S	141	LYS	CA-CB-CG	8.05	131.10	113.40
1	P	58	GLU	CA-CB-CG	8.01	131.01	113.40
2	S	42	LEU	CA-CB-CG	7.99	133.67	115.30
1	P	53	GLU	CA-CB-CG	7.96	130.92	113.40
2	S	55	THR	CA-CB-CG2	7.86	123.40	112.40
2	S	66	THR	CA-CB-CG2	7.79	123.31	112.40
2	S	195	GLU	OE1-CD-OE2	-7.75	114.00	123.30
1	P	41	PHE	CB-CG-CD2	-7.43	115.60	120.80
2	S	16	LEU	CB-CG-CD2	7.42	123.62	111.00
1	P	43	TYR	CA-CB-CG	7.31	127.30	113.40
2	S	106	TRP	CA-CB-CG	7.23	127.43	113.70
2	S	54	GLU	CA-CB-CG	7.07	128.96	113.40
2	S	8	VAL	CA-CB-CG1	7.07	121.50	110.90
2	S	71	THR	CA-CB-CG2	7.07	122.29	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	164	THR	O-C-N	-7.03	111.45	122.70
1	P	77	TYR	CA-CB-CG	7.01	126.73	113.40
2	S	63	SER	N-CA-CB	6.97	120.96	110.50
1	P	68	VAL	N-CA-CB	6.86	126.59	111.50
2	S	4	VAL	CA-CB-CG2	6.86	121.18	110.90
2	S	254	THR	CA-CB-CG2	6.84	121.97	112.40
2	S	247	ARG	CD-NE-CZ	6.78	133.10	123.60
2	S	251	GLU	OE1-CD-OE2	-6.76	115.19	123.30
2	S	28	VAL	CA-CB-CG2	6.74	121.01	110.90
2	S	203	VAL	CA-CB-CG2	6.73	121.00	110.90
2	S	212	ASN	CB-CA-C	6.63	123.67	110.40
2	S	104	TYR	CA-CB-CG	6.62	125.98	113.40
1	P	73	VAL	CA-CB-CG1	6.61	120.81	110.90
2	S	159	SER	CB-CA-C	6.61	122.65	110.10
2	S	259	ASP	CA-CB-CG	6.54	127.79	113.40
2	S	257	LEU	O-C-N	-6.54	112.09	123.20
2	S	36	ASP	CB-CG-OD2	6.52	124.17	118.30
2	S	185	GLN	CA-CB-CG	6.42	127.52	113.40
1	P	8	LYS	CA-CB-CG	6.40	127.48	113.40
2	S	21	TYR	CB-CG-CD2	-6.39	117.16	121.00
2	S	265	LYS	C-N-CA	6.38	135.70	122.30
2	S	242	THR	CA-CB-CG2	6.36	121.31	112.40
2	S	4	VAL	CA-CB-CG1	6.35	120.43	110.90
2	S	241	TRP	CA-CB-CG	6.35	125.77	113.70
2	S	62	ASN	C-N-CA	6.31	137.48	121.70
2	S	4	VAL	CG1-CB-CG2	-6.29	100.83	110.90
1	P	65	VAL	CG1-CB-CG2	-6.25	100.90	110.90
2	S	258	GLY	CA-C-O	6.23	131.81	120.60
1	P	73	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	P	56	VAL	CA-CB-CG1	6.16	120.14	110.90
2	S	6	TYR	CB-CG-CD2	-6.16	117.31	121.00
2	S	142	ALA	C-N-CA	6.14	137.06	121.70
2	S	12	LYS	O-C-N	-6.13	112.89	122.70
2	S	93	VAL	CA-CB-CG2	6.11	120.06	110.90
1	P	7	GLU	CB-CG-CD	6.11	130.69	114.20
2	S	84	VAL	CA-CB-CG1	6.09	120.04	110.90
2	S	275	GLN	CB-CA-C	6.08	122.56	110.40
2	S	145	SER	N-CA-CB	-6.03	101.46	110.50
1	P	51	LEU	CB-CG-CD1	6.01	121.22	111.00
2	S	93	VAL	CB-CA-C	6.00	122.79	111.40
2	S	140	ASP	CA-CB-CG	6.00	126.59	113.40
2	S	8	VAL	CG1-CB-CG2	-5.99	101.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	227	VAL	CA-CB-CG2	5.92	119.79	110.90
2	S	199	MET	C-N-CA	5.91	136.47	121.70
1	P	57	LYS	CB-CG-CD	5.87	126.86	111.60
2	S	207	SER	C-N-CA	5.86	136.34	121.70
2	S	251	GLU	CB-CG-CD	5.83	129.94	114.20
2	S	17	HIS	CA-CB-CG	5.78	123.42	113.60
1	P	54	LYS	CA-CB-CG	5.77	126.09	113.40
1	P	19	SER	CB-CA-C	-5.77	99.14	110.10
2	S	60	ASP	CB-CA-C	5.77	121.93	110.40
2	S	164	THR	C-N-CA	5.74	136.04	121.70
2	S	220	THR	CA-CB-CG2	5.70	120.38	112.40
1	P	39	LYS	CB-CG-CD	5.69	126.39	111.60
2	S	259	ASP	CB-CA-C	5.69	121.78	110.40
2	S	41	ASP	CA-CB-CG	5.65	125.83	113.40
2	S	135	LEU	CB-CA-C	5.64	120.91	110.20
1	P	19	SER	O-C-N	-5.59	113.76	122.70
2	S	73	LEU	N-CA-CB	-5.58	99.23	110.40
2	S	12	LYS	CB-CA-C	5.58	121.56	110.40
2	S	196	LEU	CB-CA-C	5.58	120.79	110.20
1	P	62	ASP	CB-CG-OD1	5.57	123.31	118.30
1	P	53	GLU	CB-CG-CD	5.57	129.24	114.20
2	S	115	ILE	N-CA-CB	5.54	123.55	110.80
2	S	167	TYR	CB-CG-CD1	5.52	124.31	121.00
1	P	38	GLN	CA-CB-CG	5.52	125.55	113.40
2	S	161	SER	O-C-N	-5.49	113.91	122.70
2	S	51	VAL	CA-CB-CG2	5.46	119.08	110.90
2	S	156	GLU	CB-CG-CD	5.45	128.91	114.20
1	P	68	VAL	CA-CB-CG2	5.42	119.02	110.90
2	S	84	VAL	CG1-CB-CG2	-5.40	102.27	110.90
2	S	54	GLU	CG-CD-OE1	5.40	129.09	118.30
2	S	168	PRO	N-CA-C	5.38	126.08	112.10
2	S	73	LEU	CB-CG-CD1	5.38	120.14	111.00
2	S	125	SER	CA-C-O	5.36	131.36	120.10
1	P	77	TYR	CB-CG-CD1	5.36	124.22	121.00
2	S	99	ASP	CB-CG-OD1	5.36	123.12	118.30
1	P	56	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	P	66	ALA	C-N-CA	5.35	135.08	121.70
2	S	246	VAL	CA-CB-CG1	5.34	118.90	110.90
2	S	206	VAL	CA-CB-CG1	5.33	118.90	110.90
1	P	62	ASP	CA-CB-CG	5.33	125.12	113.40
1	P	39	LYS	CA-C-O	5.32	131.26	120.10
2	S	119	MET	CA-CB-CG	5.30	122.31	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S	150	VAL	CG1-CB-CG2	-5.29	102.43	110.90
1	P	12	VAL	CG1-CB-CG2	-5.29	102.44	110.90
2	S	73	LEU	CA-CB-CG	5.29	127.46	115.30
1	P	7	GLU	CA-CB-CG	5.27	125.00	113.40
1	P	67	TYR	CB-CG-CD2	5.26	124.16	121.00
1	P	59	LEU	CA-CB-CG	5.26	127.40	115.30
1	P	73	VAL	CB-CA-C	5.26	121.39	111.40
2	S	195	GLU	CA-CB-CG	5.24	124.92	113.40
2	S	90	LEU	CB-CG-CD1	5.23	119.89	111.00
2	S	147	VAL	CA-CB-CG2	5.21	118.72	110.90
2	S	162	SER	CB-CA-C	5.21	120.00	110.10
2	S	209	LEU	CA-CB-CG	5.20	127.26	115.30
1	P	41	PHE	CA-CB-CG	5.19	126.36	113.90
2	S	36	ASP	CA-CB-CG	5.18	124.80	113.40
2	S	26	VAL	CG1-CB-CG2	-5.16	102.64	110.90
1	P	24	ALA	CB-CA-C	5.16	117.84	110.10
2	S	105	SER	C-N-CA	5.16	134.59	121.70
2	S	44	VAL	CB-CA-C	5.15	121.19	111.40
1	P	77	TYR	CA-C-O	5.15	130.91	120.10
2	S	95	VAL	CA-CB-CG1	5.15	118.62	110.90
2	S	58	PHE	CB-CG-CD1	5.13	124.39	120.80
2	S	51	VAL	CA-CB-CG1	5.10	118.55	110.90
2	S	41	ASP	C-N-CA	5.09	134.42	121.70
2	S	33	SER	N-CA-CB	-5.08	102.87	110.50
2	S	60	ASP	CA-CB-CG	5.07	124.56	113.40
2	S	253	THR	O-C-N	-5.07	114.59	122.70
2	S	30	VAL	CG1-CB-CG2	-5.07	102.80	110.90
1	P	77	TYR	CB-CA-C	5.05	120.50	110.40
2	S	68	VAL	CA-CB-CG1	5.05	118.47	110.90
2	S	208	THR	CA-CB-CG2	5.05	119.47	112.40
2	S	185	GLN	CB-CG-CD	5.05	124.72	111.60
2	S	259	ASP	N-CA-CB	-5.05	101.52	110.60
2	S	174	VAL	CA-CB-CG1	5.04	118.46	110.90
2	S	205	ILE	CA-CB-CG1	5.03	120.55	111.00
2	S	27	LYS	CA-CB-CG	5.02	124.45	113.40
2	S	74	ALA	C-N-CA	5.02	134.25	121.70
2	S	57	PRO	C-N-CA	5.01	134.24	121.70
2	S	30	VAL	CB-CA-C	5.00	120.91	111.40

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 (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	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:9:LYS:HD3	2:S:103:GLN:CD	2.34	0.48
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	11 5
2	S	262/266 (98%)	250 (95%)	11 (4%)	1 (0%)	34 30
All	All	331/344 (96%)	314 (95%)	15 (4%)	2 (1%)	25 19

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	49 (83%)	10 (17%)	2 1
2	S	197/198 (100%)	187 (95%)	10 (5%)	24 19
All	All	256/260 (98%)	236 (92%)	20 (8%)	12 8

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	16	GLN
1	P	18	MET
1	P	21	MET
1	P	22	SER
1	P	27	LYS
1	P	36	LYS
1	P	37	VAL
1	P	51	LEU
1	P	57	LYS
1	P	61	LYS
2	S	16	LEU
2	S	60	ASP
2	S	156	GLU
2	S	168	PRO
2	S	180	VAL
2	S	186	ARG
2	S	188	SER
2	S	222	MET
2	S	237	LYS
2	S	259	ASP

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	38	GLN
1	P	72	HIS
2	S	43	ASN
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 monosaccharides 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 (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.