



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:37 PM UTC

PDB ID : 8LPR / pdb_00008lpr
Title : STRUCTURAL BASIS FOR BROAD SPECIFICITY IN ALPHA-LYTIC
PROTEASE MUTANTS
Authors : Fujishige, A.; Bone, R.; Agard, D.A.
Deposited on : 1991-08-05
Resolution : 2.25 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

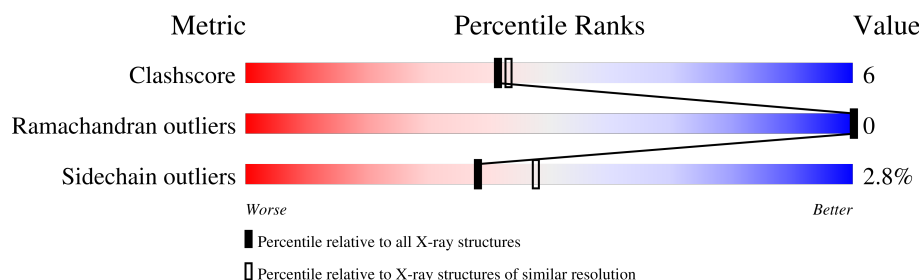
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	198	
2	P	5	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1569 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 ALPHA-LYTIC PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1388	844	262	275	7			

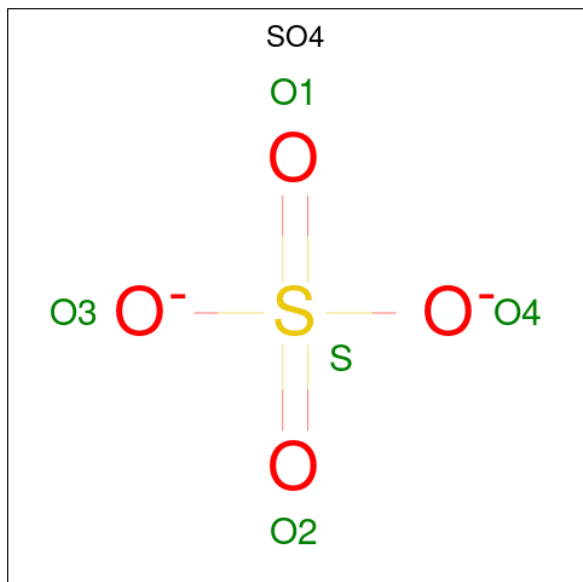
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ALA	MET	conflict	UNP P00778

- Molecule 2 is a protein called METHOXYSUCCINYL-ALA-ALA-PRO-PHENYLALANINE BORONIC ACID INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	4	Total	B	C	N	O	0	0	0
			29	1	19	4	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

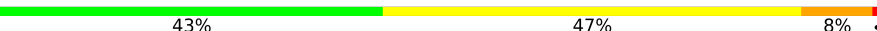
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	P	2	Total	O	0	0
			2	2		

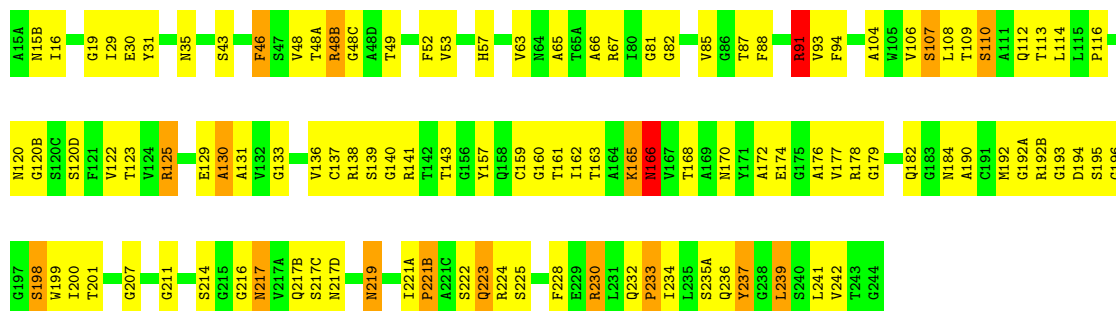
3 Residue-property plots

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.

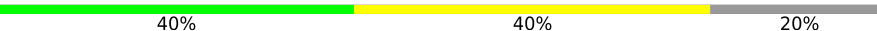
Note EDS was not executed.

• Molecule 1: ALPHA-LYTIC PROTEASE

Chain A: 



• Molecule 2: METHOXYSUCCINYL-ALA-ALA-PRO-PHENYLALANINE BORONIC ACID INHIBITOR

Chain P: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.30Å 66.30Å 80.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.25	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.132 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1569	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: SO4, B2F

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.50	3/1406 (0.2%)	2.89	172/1906 (9.0%)
2	P	1.41	0/17	3.05	2/23 (8.7%)
All	All	1.50	3/1423 (0.2%)	2.89	174/1929 (9.0%)

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	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLY	N-CA	5.61	1.51	1.45
1	A	178	ARG	NE-CZ	5.33	1.39	1.33
1	A	168	THR	CA-CB	5.01	1.60	1.53

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48(B)	ARG	NE-CZ-NH1	-15.99	105.51	121.50
1	A	48(B)	ARG	CD-NE-CZ	15.62	146.27	124.40
1	A	224	ARG	CA-C-O	-10.75	108.56	120.92
1	A	35	ASN	OD1-CG-ND2	10.21	132.81	122.60
1	A	112	GLN	OE1-CD-NE2	-10.03	112.57	122.60
1	A	106	VAL	CA-C-O	-10.02	109.86	120.48
1	A	120	ASN	OD1-CG-ND2	-9.90	112.70	122.60
2	P	3	ALA	O-C-N	9.73	129.14	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ASN	CA-CB-CG	-9.52	103.08	112.60
1	A	48(B)	ARG	NH1-CZ-NH2	9.14	131.18	119.30
1	A	192	MET	N-CA-CB	-9.09	97.48	111.56
1	A	239	LEU	CA-C-O	-8.97	110.71	121.66
1	A	120(D)	SER	N-CA-CB	-8.79	95.01	110.14
1	A	139	SER	N-CA-CB	-8.78	95.42	111.13
1	A	192(B)	ARG	NE-CZ-NH2	-8.64	111.42	119.20
1	A	235(A)	SER	O-C-N	8.46	131.23	122.09
1	A	120	ASN	CA-CB-CG	-8.27	104.33	112.60
1	A	110	SER	CA-CB-OG	-8.24	94.62	111.10
1	A	184	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	A	48(A)	THR	CA-C-O	-7.92	112.17	121.44
1	A	31	TYR	CA-C-O	-7.90	111.89	121.06
1	A	184	ASN	O-C-N	7.86	132.44	122.22
1	A	113	THR	O-C-N	7.83	133.00	123.13
1	A	225	SER	CA-CB-OG	-7.78	95.54	111.10
1	A	123	THR	CA-C-O	-7.71	111.90	120.69
1	A	224	ARG	O-C-N	7.64	132.03	123.16
1	A	201	THR	CA-CB-OG1	-7.63	98.16	109.60
1	A	177	VAL	N-CA-CB	7.56	121.78	112.10
1	A	123	THR	O-C-N	7.54	131.87	123.04
1	A	48(C)	GLY	N-CA-C	-7.53	98.52	111.47
1	A	217	ASN	CA-C-O	7.49	128.71	120.92
1	A	176	ALA	CA-C-N	7.42	133.35	123.11
1	A	176	ALA	C-N-CA	7.42	133.35	123.11
1	A	113	THR	CA-C-O	-7.35	112.59	120.46
1	A	16	ILE	CA-C-O	-7.32	111.82	120.75
1	A	57	HIS	CA-C-O	-7.29	109.58	119.05
1	A	225	SER	CA-C-O	-7.20	112.55	120.33
1	A	139	SER	CA-CB-OG	-7.18	96.74	111.10
1	A	67	ARG	O-C-N	7.16	132.01	123.27
1	A	217	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	A	110	SER	N-CA-CB	-7.14	99.22	110.22
1	A	93	VAL	O-C-N	7.11	130.35	123.03
1	A	125	ARG	NH1-CZ-NH2	7.09	128.51	119.30
1	A	241	LEU	N-CA-CB	-7.07	99.57	109.97
1	A	43	SER	CA-C-O	-7.07	113.12	121.11
1	A	178	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	A	235(A)	SER	CA-C-O	-7.00	113.49	120.70
1	A	35	ASN	CA-CB-CG	-6.98	105.62	112.60
1	A	48(B)	ARG	CB-CG-CD	-6.97	95.27	111.30
2	P	4	ALA	CB-CA-C	-6.90	100.15	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	GLY	O-C-N	6.88	130.53	123.92
1	A	67	ARG	NE-CZ-NH1	6.79	128.29	121.50
1	A	222	SER	CA-C-O	-6.79	112.43	120.10
1	A	67	ARG	CA-C-O	-6.77	112.87	120.66
1	A	190	ALA	CA-C-O	-6.75	113.70	121.47
1	A	91	ARG	CD-NE-CZ	6.75	133.85	124.40
1	A	48(B)	ARG	CB-CA-C	6.73	121.11	111.82
1	A	85	VAL	CA-C-O	-6.72	112.06	118.98
1	A	109	THR	CA-C-N	6.68	129.91	120.28
1	A	109	THR	C-N-CA	6.68	129.91	120.28
1	A	161	THR	CA-CB-CG2	6.67	121.85	110.50
1	A	192(B)	ARG	CB-CG-CD	-6.67	95.95	111.30
1	A	211	GLY	O-C-N	6.60	130.25	123.92
1	A	182	GLN	CB-CG-CD	-6.58	101.41	112.60
1	A	107	SER	CA-CB-OG	-6.56	97.98	111.10
1	A	184	ASN	CA-C-O	-6.56	112.01	119.95
1	A	190	ALA	N-CA-C	-6.54	100.80	110.48
1	A	162	ILE	O-C-N	6.52	130.04	122.81
1	A	200	ILE	CA-C-O	-6.49	114.96	121.45
1	A	236	GLN	CG-CD-NE2	-6.44	106.74	116.40
1	A	236	GLN	CG-CD-OE1	6.44	133.67	120.80
1	A	163	THR	O-C-N	6.36	130.17	122.48
1	A	53	VAL	O-C-N	6.33	129.91	122.69
1	A	143	THR	CA-C-O	-6.33	111.94	119.35
1	A	230	ARG	CA-C-O	-6.32	114.23	121.19
1	A	91	ARG	NH1-CZ-NH2	-6.32	111.08	119.30
1	A	131	ALA	CA-C-O	-6.29	113.90	121.89
1	A	224	ARG	NE-CZ-NH2	-6.27	113.56	119.20
1	A	242	VAL	N-CA-CB	-6.24	103.73	110.53
1	A	143	THR	CA-CB-CG2	6.19	121.02	110.50
1	A	108	LEU	N-CA-CB	-6.17	100.93	110.56
1	A	230	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	A	15(B)	ASN	CB-CG-ND2	6.15	125.63	116.40
1	A	165	LYS	CA-C-O	-6.11	114.31	121.46
1	A	15(B)	ASN	O-C-N	6.11	130.17	123.27
1	A	214	SER	O-C-N	6.10	129.85	121.92
1	A	91	ARG	NE-CZ-NH2	6.10	124.69	119.20
1	A	174	GLU	CG-CD-OE2	-6.05	104.48	118.40
1	A	161	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	94	PHE	CA-CB-CG	-5.99	107.81	113.80
1	A	237	TYR	CA-C-O	-5.98	112.35	119.35
1	A	141	ARG	NE-CZ-NH2	5.96	124.56	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	PRO	CB-CA-C	5.93	121.45	112.21
1	A	109	THR	N-CA-C	-5.89	103.16	110.41
1	A	166	ASN	CB-CG-ND2	5.89	125.23	116.40
1	A	217(D)	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	93	VAL	N-CA-CB	5.85	120.65	111.99
1	A	163	THR	CA-C-O	-5.85	112.71	118.97
1	A	120(D)	SER	CA-CB-OG	-5.85	99.41	111.10
1	A	15(B)	ASN	N-CA-C	-5.84	99.72	109.24
1	A	221(B)	PRO	CA-C-O	-5.83	114.69	121.34
1	A	223	GLN	CA-C-O	-5.81	112.74	119.59
1	A	15(B)	ASN	CA-C-N	-5.80	115.12	122.43
1	A	15(B)	ASN	C-N-CA	-5.80	115.12	122.43
1	A	224	ARG	CD-NE-CZ	-5.76	116.33	124.40
1	A	29	ILE	CB-CA-C	5.76	117.93	111.59
1	A	178	ARG	N-CA-CB	-5.76	101.54	110.46
1	A	184	ASN	CA-CB-CG	-5.75	106.85	112.60
1	A	114	LEU	CA-C-O	-5.74	114.15	120.69
1	A	196	GLY	CA-C-O	-5.72	113.54	119.20
1	A	63	VAL	CB-CA-C	5.70	120.92	111.51
1	A	178	ARG	CD-NE-CZ	-5.69	116.43	124.40
1	A	133	GLY	CA-C-O	-5.67	113.20	119.27
1	A	57	HIS	O-C-N	5.67	130.28	122.46
1	A	49	THR	CA-CB-OG1	-5.65	101.13	109.60
1	A	130	ALA	CA-C-O	5.65	128.47	121.81
1	A	217	ASN	O-C-N	-5.64	113.67	122.70
1	A	195	SER	CB-CA-C	-5.61	100.67	109.70
1	A	30	GLU	CB-CG-CD	-5.60	103.07	112.60
1	A	195	SER	CA-C-O	-5.60	114.99	121.15
1	A	222	SER	N-CA-CB	5.60	118.84	110.22
1	A	120(B)	GLY	CA-C-O	5.58	129.16	121.46
1	A	157	TYR	N-CA-CB	-5.56	101.35	110.42
1	A	225	SER	O-C-N	5.56	130.46	123.12
1	A	65	ALA	N-CA-C	-5.56	102.79	110.35
1	A	228	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	66	ALA	CA-C-O	-5.54	114.65	120.80
1	A	219	ASN	N-CA-C	-5.53	105.23	112.41
1	A	112	GLN	CG-CD-NE2	5.50	124.66	116.40
1	A	113	THR	CA-CB-OG1	-5.49	101.37	109.60
1	A	141	ARG	NE-CZ-NH1	-5.48	116.02	121.50
1	A	182	GLN	CA-C-N	5.47	126.42	121.82
1	A	182	GLN	C-N-CA	5.47	126.42	121.82
1	A	166	ASN	CA-CB-CG	-5.46	107.14	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SER	N-CA-C	5.42	118.30	110.28
1	A	199	TRP	N-CA-C	-5.42	99.58	108.41
1	A	234	ILE	CA-C-O	-5.41	115.12	120.85
1	A	19	GLY	CA-C-O	-5.38	113.67	119.27
1	A	217(B)	GLN	CB-CG-CD	5.38	121.75	112.60
1	A	48	VAL	CA-C-O	-5.37	116.07	121.49
1	A	123	THR	CA-CB-OG1	-5.37	101.55	109.60
1	A	236	GLN	CA-CB-CG	-5.36	103.38	114.10
1	A	216	GLY	CA-C-O	-5.36	115.73	121.35
1	A	224	ARG	CB-CA-C	-5.35	100.70	109.53
1	A	136	VAL	N-CA-CB	-5.34	101.05	112.00
1	A	193	GLY	O-C-N	-5.34	116.79	122.56
1	A	133	GLY	O-C-N	5.27	128.60	122.65
1	A	237	TYR	O-C-N	5.26	128.92	122.34
1	A	221(B)	PRO	O-C-N	5.25	131.11	122.70
1	A	46	PHE	CA-C-N	5.22	128.26	120.95
1	A	46	PHE	C-N-CA	5.22	128.26	120.95
1	A	122	VAL	N-CA-C	-5.21	100.24	107.80
1	A	110	SER	CB-CA-C	-5.21	100.99	110.63
1	A	109	THR	CA-CB-OG1	-5.21	101.79	109.60
1	A	82	GLY	CA-C-O	-5.21	113.80	118.95
1	A	125	ARG	NE-CZ-NH1	-5.21	116.30	121.50
1	A	174	GLU	N-CA-C	5.19	119.46	113.18
1	A	217(C)	SER	N-CA-CB	5.18	119.00	110.39
1	A	81	GLY	O-C-N	5.18	129.43	122.70
1	A	160	GLY	O-C-N	5.14	129.39	122.70
1	A	192(B)	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	207	GLY	O-C-N	5.13	128.46	122.45
1	A	125	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	217	ASN	CB-CG-OD1	5.10	131.01	120.80
1	A	172	ALA	CA-C-O	-5.09	114.34	120.10
1	A	109	THR	CA-C-O	5.09	127.79	121.99
1	A	116	PRO	CA-C-O	-5.09	117.54	121.31
1	A	198	SER	CA-C-O	-5.08	115.47	121.16
1	A	87	THR	CA-C-O	5.08	127.14	121.40
1	A	35	ASN	N-CA-CB	-5.06	104.73	112.28
1	A	224	ARG	CB-CG-CD	-5.06	99.65	111.30
1	A	222	SER	O-C-N	5.06	128.13	122.22
1	A	178	ARG	CA-CB-CG	-5.02	104.06	114.10
1	A	88	PHE	CA-C-O	-5.02	114.76	120.58

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	ARG	Sidechain
1	A	230	ARG	Sidechain

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	1388	0	1356	18	0
2	P	29	0	26	0	0
3	A	5	0	0	0	0
4	A	145	0	0	2	0
4	P	2	0	0	0	0
All	All	1569	0	1382	18	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 6.

All (18) 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:166:ASN:HD22	1:A:179:GLY:HA2	1.63	0.62
1:A:221(B):PRO:HG2	1:A:223:GLN:NE2	2.17	0.60
1:A:46:PHE:O	1:A:52:PHE:HA	2.05	0.56
1:A:137:CYS:HA	1:A:159:CYS:HA	1.90	0.52
1:A:129:GLU:HG3	4:A:365:HOH:O	2.13	0.48
1:A:48(B):ARG:HG3	1:A:239:LEU:HD23	1.96	0.48
1:A:221(A):ILE:HB	1:A:221(B):PRO:HD2	1.96	0.47
1:A:138:ARG:HA	1:A:198:SER:O	2.16	0.46
1:A:237:TYR:HB2	1:A:239:LEU:HG	2.00	0.44
1:A:217:ASN:O	1:A:219:ASN:HB3	2.17	0.44
1:A:130:ALA:O	1:A:165:LYS:NZ	2.44	0.43
1:A:48(B):ARG:HD2	4:A:356:HOH:O	2.19	0.41
1:A:166:ASN:ND2	1:A:179:GLY:HA2	2.33	0.41
1:A:166:ASN:HA	1:A:179:GLY:HA2	2.03	0.41
1:A:232:GLN:N	1:A:233:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HB3	1:A:104:ALA:HB2	2.03	0.41
1:A:192(A):GLY:O	1:A:194:ASP:HB2	2.21	0.41
1:A:221(B):PRO:HG2	1:A:223:GLN:CD	2.46	0.41

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	A	196/198 (99%)	185 (94%)	11 (6%)	0	100	100
2	P	2/5 (40%)	2 (100%)	0	0	100	100
All	All	198/203 (98%)	187 (94%)	11 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	A	141/141 (100%)	137 (97%)	4 (3%)	38	48
2	P	1/1 (100%)	1 (100%)	0	100	100
All	All	142/142 (100%)	138 (97%)	4 (3%)	38	48

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	ARG
1	A	107	SER
1	A	110	SER
1	A	166	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	166	ASN
1	A	223	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	B2F	P	1	2,1	7,12,12	0.96	0	8,15,15	0.71	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
2	B2F	P	1	2,1	-	2/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	1	B2F	CA-CB-CG-CD1
2	P	1	B2F	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
3	SO4	A	1	-	4,4,4	0.72	0	6,6,6	0.76	0

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.