



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:05 PM UTC

PDB ID : 2PSG / pdb_00002psg
Title : REFINED STRUCTURE OF PORCINE PEPSINOGEN AT 1.8
ANGSTROMS RESOLUTION
Authors : James, M.N.G.; Sielecki, A.R.
Deposited on : 1991-01-23
Resolution : 1.80 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

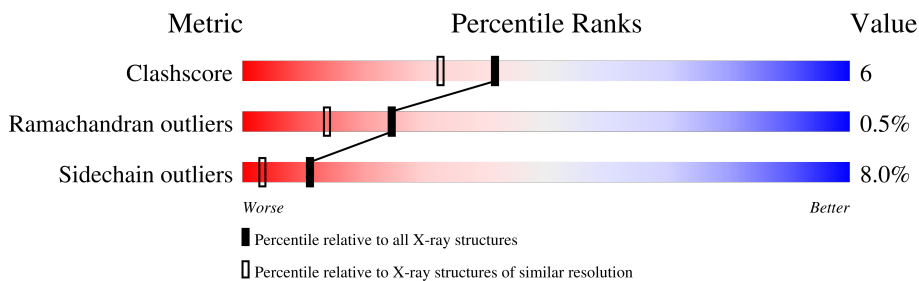
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	370	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3031 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 PEPSINOGEN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	P	S	0	1	0
			2794	1766	432	585	1	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19P	ASP	ASN	conflict	UNP P00791
A	?	-	ILE	deletion	UNP P00791
A	263	ASP	ASN	conflict	UNP P00791

- Molecule 2 is water.

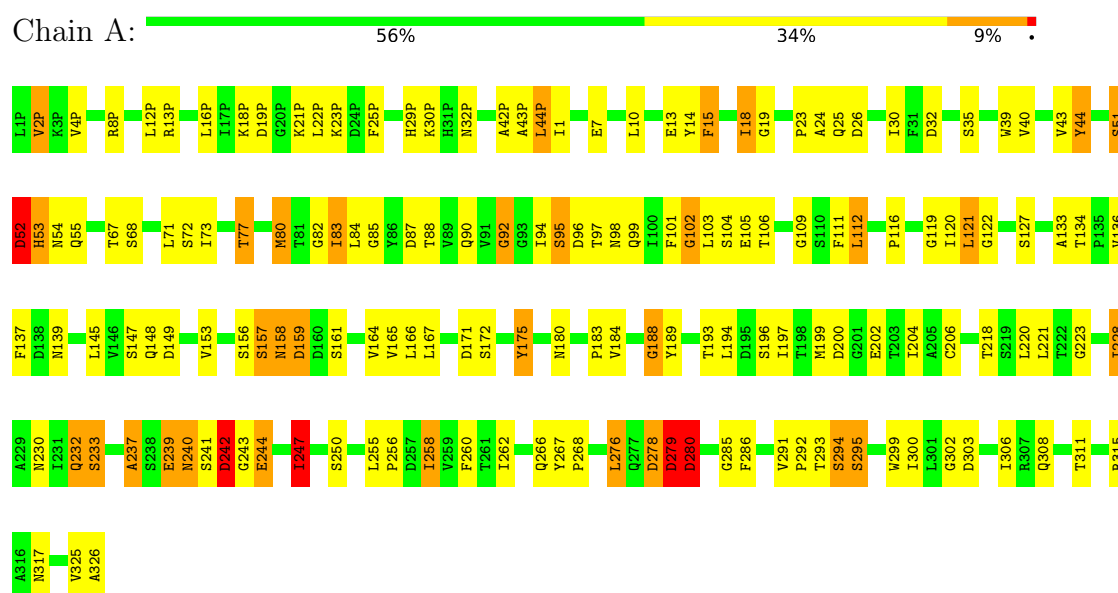
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	237	Total	O	0	0
			237	237		

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: PEPSINOGEN



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.78Å 43.41Å 88.58Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	8.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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: SEP

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	1.35	8/2850 (0.3%)	2.47	199/3889 (5.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	GLY	N-CA	9.16	1.53	1.45
1	A	165	VAL	CA-C	7.50	1.62	1.52
1	A	97	THR	CA-CB	5.99	1.62	1.53
1	A	121	LEU	C-N	-5.80	1.28	1.33
1	A	25	GLN	N-CA	5.43	1.52	1.46
1	A	2(P)	VAL	CA-C	5.38	1.59	1.52
1	A	14	TYR	N-CA	5.30	1.52	1.46
1	A	112	LEU	N-CA	5.10	1.52	1.46

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	ASN	CA-CB-CG	14.86	127.46	112.60
1	A	180	ASN	CA-CB-CG	11.49	124.09	112.60
1	A	244	GLU	N-CA-C	11.44	127.12	110.42
1	A	311	THR	O-C-N	10.89	136.26	123.30
1	A	165	VAL	N-CA-CB	10.81	125.09	111.46
1	A	148	GLN	O-C-N	10.59	135.99	123.17
1	A	53	HIS	CA-CB-CG	-10.12	103.69	113.80
1	A	2(P)	VAL	O-C-N	9.50	134.55	122.77
1	A	102	GLY	CA-C-O	9.31	131.28	121.23
1	A	148	GLN	OE1-CD-NE2	9.07	131.67	122.60
1	A	223	GLY	O-C-N	8.94	130.71	121.77
1	A	22(P)	LEU	CA-C-O	-8.83	111.60	120.70
1	A	161	SER	N-CA-C	-8.83	95.95	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ILE	O-C-N	8.81	130.42	121.87
1	A	280	ASP	CA-CB-CG	8.73	121.33	112.60
1	A	19(P)	ASP	CA-CB-CG	-8.71	103.89	112.60
1	A	189	TYR	N-CA-C	-8.57	97.78	110.46
1	A	202	GLU	O-C-N	8.39	132.89	123.16
1	A	220	LEU	N-CA-C	8.39	123.42	110.42
1	A	243	GLY	CA-C-N	8.35	134.59	121.56
1	A	243	GLY	C-N-CA	8.35	134.59	121.56
1	A	262	ILE	O-C-N	8.33	131.84	123.18
1	A	317	ASN	OD1-CG-ND2	8.23	130.83	122.60
1	A	204	ILE	CA-C-O	-8.15	111.65	118.98
1	A	52	ASP	CA-CB-CG	-8.07	104.53	112.60
1	A	137	PHE	CA-CB-CG	-8.06	105.74	113.80
1	A	92	GLY	O-C-N	8.00	130.25	122.41
1	A	158	ASN	N-CA-CB	-7.91	99.25	111.74
1	A	311	THR	CA-C-N	-7.83	113.49	123.19
1	A	311	THR	C-N-CA	-7.83	113.49	123.19
1	A	165	VAL	N-CA-C	-7.80	96.48	107.80
1	A	54	ASN	O-C-N	-7.74	113.44	122.89
1	A	18	ILE	CA-C-N	-7.72	116.85	122.18
1	A	18	ILE	C-N-CA	-7.72	116.85	122.18
1	A	13	GLU	O-C-N	7.68	130.10	122.19
1	A	184	VAL	N-CA-C	-7.61	98.84	108.89
1	A	109	GLY	O-C-N	-7.54	113.89	122.56
1	A	180	ASN	OD1-CG-ND2	-7.54	115.06	122.60
1	A	13(P)	ARG	NE-CZ-NH2	7.46	125.92	119.20
1	A	266	GLN	OE1-CD-NE2	7.46	130.06	122.60
1	A	105	GLU	O-C-N	7.46	131.20	122.25
1	A	242	ASP	N-CA-C	-7.42	98.21	109.79
1	A	120	ILE	O-C-N	7.41	131.03	123.10
1	A	25(P)	PHE	CA-CB-CG	-7.37	106.43	113.80
1	A	111	PHE	CA-C-O	-7.33	111.81	120.10
1	A	233	SER	CB-CA-C	7.21	123.10	110.85
1	A	98	ASN	O-C-N	7.17	131.45	122.55
1	A	171	ASP	CA-CB-CG	7.16	119.76	112.60
1	A	22(P)	LEU	N-CA-C	6.92	118.61	111.14
1	A	119	GLY	O-C-N	6.89	132.10	123.56
1	A	303	ASP	CA-C-O	-6.84	113.25	120.63
1	A	32	ASP	N-CA-C	6.83	120.44	107.75
1	A	13(P)	ARG	CA-C-N	6.82	129.42	120.28
1	A	13(P)	ARG	C-N-CA	6.82	129.42	120.28
1	A	83	ILE	N-CA-CB	-6.77	101.06	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLN	CA-C-O	-6.76	112.88	120.66
1	A	145	LEU	CA-C-O	-6.72	111.19	119.18
1	A	266	GLN	CA-CB-CG	-6.71	100.67	114.10
1	A	13	GLU	CA-C-N	-6.68	112.91	122.94
1	A	13	GLU	C-N-CA	-6.68	112.91	122.94
1	A	148	GLN	CA-C-O	-6.68	113.85	121.40
1	A	326	ALA	N-CA-CB	6.66	120.39	110.40
1	A	44	TYR	CA-CB-CG	-6.66	101.92	113.90
1	A	55	GLN	O-C-N	6.60	131.32	123.27
1	A	294	SER	N-CA-C	-6.58	103.80	110.97
1	A	109	GLY	N-CA-C	-6.56	104.54	112.48
1	A	84	LEU	O-C-N	6.55	130.86	123.19
1	A	88	THR	CA-CB-OG1	-6.54	99.80	109.60
1	A	10	LEU	O-C-N	6.50	129.02	122.12
1	A	149	ASP	O-C-N	6.50	131.19	122.61
1	A	147	SER	N-CA-C	6.49	118.35	111.28
1	A	95	SER	CA-C-O	6.45	127.81	120.84
1	A	44(P)	LEU	CB-CA-C	6.45	121.00	110.88
1	A	19	GLY	N-CA-C	-6.44	99.92	111.19
1	A	111	PHE	O-C-N	6.40	129.71	122.22
1	A	2(P)	VAL	CA-C-O	-6.39	112.96	120.75
1	A	267	TYR	O-C-N	6.38	127.29	121.04
1	A	317	ASN	O-C-N	6.38	129.96	122.24
1	A	302	GLY	CA-C-N	6.33	129.05	120.38
1	A	302	GLY	C-N-CA	6.33	129.05	120.38
1	A	122	GLY	CA-C-O	-6.32	115.04	120.98
1	A	13(P)	ARG	CD-NE-CZ	6.28	133.20	124.40
1	A	197	ILE	CA-C-O	-6.25	113.96	120.27
1	A	291	VAL	O-C-N	6.25	128.22	121.10
1	A	120	ILE	CA-C-O	-6.24	113.68	120.67
1	A	133	ALA	N-CA-C	-6.23	101.06	110.28
1	A	51	SER	CA-C-N	-6.23	113.94	123.47
1	A	51	SER	C-N-CA	-6.23	113.94	123.47
1	A	218	THR	CA-CB-OG1	-6.22	100.27	109.60
1	A	258	ILE	N-CA-C	-6.22	99.47	108.17
1	A	230	ASN	CA-C-O	6.19	127.32	120.82
1	A	24	ALA	O-C-N	6.16	130.40	122.89
1	A	175	TYR	O-C-N	6.16	130.18	123.10
1	A	202	GLU	CA-C-O	-6.15	113.85	120.92
1	A	278	ASP	CA-CB-CG	-6.14	106.45	112.60
1	A	54	ASN	CA-CB-CG	-6.13	106.47	112.60
1	A	4(P)	VAL	O-C-N	6.11	126.55	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	GLU	CA-C-O	-6.11	114.07	120.55
1	A	4(P)	VAL	N-CA-C	-6.09	101.08	107.60
1	A	67	THR	N-CA-CB	6.08	121.84	111.50
1	A	119	GLY	CA-C-O	-6.08	115.67	121.38
1	A	294	SER	CA-C-N	6.05	129.72	120.82
1	A	294	SER	C-N-CA	6.05	129.72	120.82
1	A	40	VAL	N-CA-C	-6.04	102.18	109.01
1	A	55	GLN	OE1-CD-NE2	-6.00	116.60	122.60
1	A	325	VAL	N-CA-CB	5.95	123.20	110.64
1	A	15	PHE	CA-CB-CG	-5.95	107.85	113.80
1	A	161	SER	CB-CA-C	5.93	119.52	109.50
1	A	279	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	83	ILE	CA-C-O	-5.91	115.46	121.67
1	A	285	GLY	O-C-N	-5.90	114.19	122.27
1	A	14	TYR	O-C-N	5.89	130.89	123.23
1	A	106	THR	CA-CB-CG2	5.89	120.52	110.50
1	A	112	LEU	CA-C-O	5.89	126.75	120.10
1	A	206	CYS	N-CA-CB	-5.86	103.03	111.70
1	A	136	VAL	CA-C-O	-5.85	115.18	121.27
1	A	32	ASP	N-CA-CB	-5.85	100.74	110.39
1	A	29(P)	HIS	O-C-N	5.85	130.05	123.27
1	A	87	ASP	N-CA-CB	5.84	120.47	111.24
1	A	232	GLN	O-C-N	5.84	128.31	122.12
1	A	19	GLY	O-C-N	-5.83	118.00	123.25
1	A	12(P)	LEU	N-CA-C	-5.83	104.93	111.28
1	A	149	ASP	CA-C-O	-5.82	114.64	122.44
1	A	73	ILE	O-C-N	5.80	129.28	123.18
1	A	80	MET	N-CA-C	-5.80	99.55	109.24
1	A	306	ILE	O-C-N	-5.77	116.04	121.87
1	A	139	ASN	OD1-CG-ND2	5.76	128.36	122.60
1	A	255	LEU	CB-CA-C	5.75	118.52	109.37
1	A	4(P)	VAL	CA-C-O	-5.75	113.62	119.89
1	A	98	ASN	CA-C-O	-5.75	115.17	121.84
1	A	167	LEU	CA-C-O	-5.75	113.99	120.43
1	A	157	SER	O-C-N	5.75	129.83	123.16
1	A	268	PRO	CA-C-N	5.74	131.10	123.00
1	A	268	PRO	C-N-CA	5.74	131.10	123.00
1	A	77	THR	N-CA-C	5.73	118.22	110.88
1	A	26	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	239	GLU	CA-C-O	-5.72	114.24	120.81
1	A	16(P)	LEU	N-CA-C	-5.70	104.98	111.14
1	A	221	LEU	N-CA-C	-5.68	99.93	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ILE	N-CA-CB	5.66	119.03	111.90
1	A	308	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	220	LEU	O-C-N	5.65	129.42	123.03
1	A	268	PRO	O-C-N	-5.61	116.06	123.13
1	A	243	GLY	N-CA-C	5.60	120.58	113.24
1	A	247	ILE	CA-C-O	-5.57	114.81	121.28
1	A	121	LEU	CA-C-N	5.56	126.33	120.43
1	A	121	LEU	C-N-CA	5.56	126.33	120.43
1	A	43	VAL	N-CA-C	-5.54	104.29	112.04
1	A	183	PRO	CB-CA-C	-5.51	103.77	110.98
1	A	83	ILE	CB-CG1-CD1	-5.49	102.28	113.80
1	A	311	THR	CA-C-O	-5.45	114.48	120.36
1	A	228	ILE	CA-C-O	-5.44	115.29	120.95
1	A	153	VAL	O-C-N	5.44	129.07	123.20
1	A	42(P)	ALA	CA-C-N	5.41	128.53	120.90
1	A	42(P)	ALA	C-N-CA	5.41	128.53	120.90
1	A	295	SER	N-CA-C	5.41	117.28	110.24
1	A	243	GLY	CA-C-O	5.41	126.25	120.40
1	A	188	GLY	N-CA-C	-5.41	100.36	113.18
1	A	99	GLN	CA-C-O	-5.40	114.38	120.43
1	A	291	VAL	CA-C-O	-5.40	112.72	119.95
1	A	15	PHE	O-C-N	5.38	129.68	123.17
1	A	202	GLU	CB-CA-C	-5.37	100.66	109.53
1	A	29(P)	HIS	CA-C-O	-5.37	114.83	121.06
1	A	193	THR	CA-C-O	5.36	126.27	120.43
1	A	25	GLN	N-CA-C	-5.33	100.48	109.07
1	A	127	SER	CA-C-O	-5.32	113.05	119.49
1	A	300	ILE	N-CA-CB	5.32	118.16	111.46
1	A	51	SER	O-C-N	5.32	129.13	122.86
1	A	54	ASN	N-CA-C	-5.29	102.46	110.28
1	A	242	ASP	N-CA-CB	5.28	118.05	110.45
1	A	260	PHE	CA-C-O	-5.27	114.69	120.43
1	A	196	SER	O-C-N	-5.27	118.31	123.26
1	A	35	SER	CA-C-N	-5.26	113.79	121.99
1	A	35	SER	C-N-CA	-5.26	113.79	121.99
1	A	299	TRP	CA-C-O	-5.26	115.17	121.11
1	A	72	SER	N-CA-CB	5.25	118.82	110.84
1	A	96	ASP	CB-CG-OD1	5.24	130.45	118.40
1	A	134	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	286	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	22(P)	LEU	O-C-N	5.22	127.73	122.09
1	A	92	GLY	CA-C-O	-5.22	113.48	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	SER	CA-C-O	-5.21	113.19	119.49
1	A	32(P)	ASN	O-C-N	5.20	127.50	121.47
1	A	164	VAL	CB-CA-C	-5.15	101.22	110.48
1	A	156	SER	CA-C-O	5.13	127.87	121.81
1	A	101	PHE	CA-C-N	-5.13	116.84	122.38
1	A	101	PHE	C-N-CA	-5.13	116.84	122.38
1	A	311	THR	N-CA-C	5.13	117.26	108.90
1	A	137	PHE	CD1-CG-CD2	5.13	126.29	118.60
1	A	7	GLU	CB-CG-CD	-5.12	103.89	112.60
1	A	180	ASN	N-CA-C	-5.12	100.90	109.24
1	A	139	ASN	CA-C-N	5.11	127.09	120.44
1	A	139	ASN	C-N-CA	5.11	127.09	120.44
1	A	315	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	237	ALA	CA-C-O	-5.07	115.64	121.47
1	A	83	ILE	O-C-N	5.05	128.64	123.04
1	A	83	ILE	CA-CB-CG2	5.05	119.08	110.50
1	A	73	ILE	CB-CG1-CD1	5.04	124.38	113.80
1	A	303	ASP	N-CA-CB	5.03	117.61	110.06

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	2794	0	2649	35	0
2	A	237	0	0	1	0
All	All	3031	0	2649	35	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 (35) 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:90:GLN:HE22	1:A:95:SER:HA	1.48	0.77
1:A:90:GLN:NE2	1:A:95:SER:HA	2.09	0.67
1:A:199:MET:CE	1:A:258:ILE:HB	2.33	0.59
1:A:239:GLU:HA	1:A:244:GLU:O	2.03	0.58
1:A:278:ASP:O	1:A:279:ASP:C	2.49	0.56
1:A:240:ASN:N	1:A:240:ASN:HD22	2.06	0.53
1:A:121:LEU:C	1:A:121:LEU:HD23	2.34	0.52
1:A:158:ASN:O	1:A:159:ASP:OD1	2.28	0.52
1:A:237:ALA:HA	1:A:247:ILE:HG13	1.93	0.51
1:A:240:ASN:ND2	1:A:244:GLU:HB2	2.26	0.50
1:A:21(P):LYS:HE2	2:A:485:HOH:O	2.11	0.50
1:A:159:ASP:O	1:A:159:ASP:CG	2.55	0.49
1:A:292:PRO:O	1:A:295:SER:HB3	2.13	0.49
1:A:71:LEU:HD22	1:A:102:GLY:HA3	1.93	0.49
1:A:2(P):VAL:HG13	1:A:92:GLY:O	2.13	0.48
1:A:8(P):ARG:HH11	1:A:159:ASP:H	1.61	0.48
1:A:240:ASN:HD22	1:A:240:ASN:H	1.60	0.48
1:A:157:SER:O	1:A:158:ASN:HB3	2.14	0.47
1:A:15:PHE:CZ	1:A:116:PRO:HG2	2.50	0.47
1:A:90:GLN:HE22	1:A:95:SER:CA	2.22	0.46
1:A:228:ILE:O	1:A:232:GLN:HG2	2.16	0.45
1:A:8(P):ARG:HD3	1:A:159:ASP:CB	2.47	0.45
1:A:8(P):ARG:HD3	1:A:159:ASP:HB2	1.98	0.45
1:A:172:SER:HA	1:A:175:TYR:CE1	2.51	0.45
1:A:276:LEU:HD23	1:A:276:LEU:N	2.32	0.44
1:A:82:GLY:HA3	1:A:103:LEU:O	2.18	0.43
1:A:43(P):ALA:HB3	1:A:77:THR:HA	2.00	0.43
1:A:199:MET:HE3	1:A:258:ILE:HB	2.00	0.42
1:A:39:TRP:CZ2	1:A:80:MET:HE1	2.55	0.42
1:A:279:ASP:OD1	1:A:280:ASP:OD1	2.38	0.42
1:A:53:HIS:NE2	1:A:112:LEU:O	2.49	0.42
1:A:240:ASN:O	1:A:242:ASP:O	2.37	0.41
1:A:51:SER:O	1:A:52:ASP:HB2	2.21	0.41
1:A:199:MET:HE2	1:A:258:ILE:HB	2.02	0.41
1:A:94:ILE:HD13	1:A:94:ILE:HG21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	368/370 (100%)	360 (98%)	6 (2%)	2 (0%)	24 14

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	ASP
1	A	188	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	314/313 (100%)	289 (92%)	25 (8%)	11 3

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18(P)	LYS
1	A	23(P)	LYS
1	A	30(P)	LYS
1	A	44(P)	LEU
1	A	18	ILE
1	A	23	PRO
1	A	30	ILE
1	A	44	TYR
1	A	52	ASP

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Mol	Chain	Res	Type
1	A	83	ILE
1	A	104	SER
1	A	159	ASP
1	A	166	LEU
1	A	194	LEU
1	A	200	ASP
1	A	233	SER
1	A	240	ASN
1	A	241	SER
1	A	242	ASP
1	A	247	ILE
1	A	256	PRO
1	A	276	LEU
1	A	280	ASP
1	A	293	THR
1	A	294	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	98	ASN
1	A	99	GLN
1	A	143	GLN
1	A	191	GLN
1	A	211	GLN
1	A	240	ASN
1	A	318	ASN

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	$\# Z > 2$
1	SEP	A	68	1	8,9,10	1.11	1 (12%)	7,12,14	3.60	2 (28%)

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
1	SEP	A	68	1	-	2/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	SEP	P-OG	-2.45	1.52	1.60

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	SEP	OG-P-O1P	7.19	125.88	106.44
1	A	68	SEP	O2P-P-OG	-5.85	91.41	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	68	SEP	C-CA-CB-OG
1	A	68	SEP	CB-OG-P-O3P

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

There are no ligands in this entry.

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.