



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:16 PM UTC

PDB ID : 1PHO / pdb_00001pho
Title : CRYSTAL STRUCTURES EXPLAIN FUNCTIONAL PROPERTIES OF TWO E. COLI PORINS
Authors : Schirmer, T.; Cowan, S.W.; Jansonius, J.N.
Deposited on : 1993-01-15
Resolution : 3.00 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

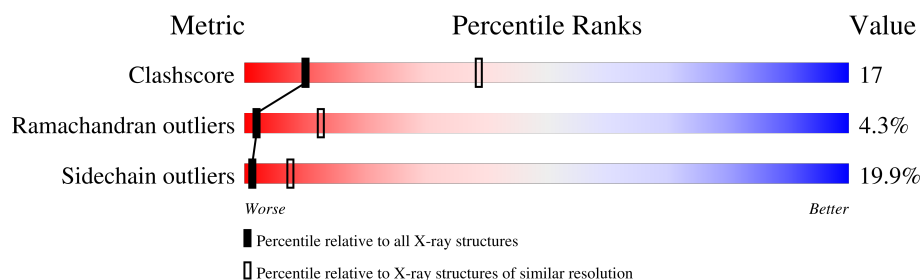
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	A	330	36% 41% 18% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2602 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 PHOSPHOPORIN.

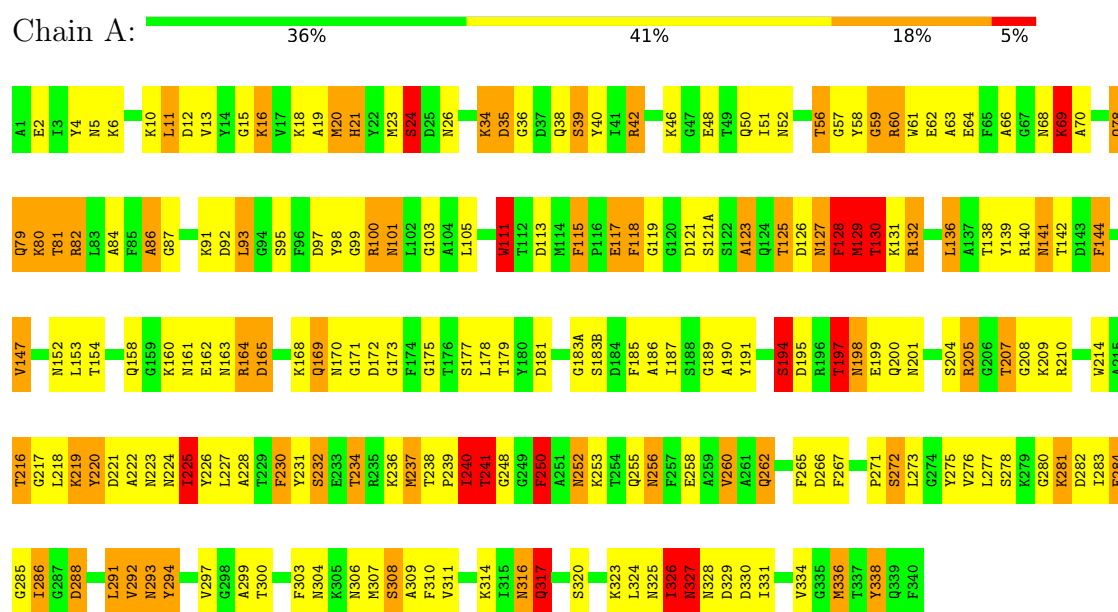
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2602	1631	437	527	7	203	0	0

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: PHOSPHOPORIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.90Å 119.90Å 51.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2602	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.36	15/2654 (0.6%)	2.38	172/3575 (4.8%)

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 (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	THR	CA-CB	8.04	1.67	1.53
1	A	241	THR	CA-CB	7.33	1.64	1.53
1	A	12	ASP	CA-CB	-6.44	1.43	1.53
1	A	81	THR	CA-CB	6.23	1.63	1.53
1	A	93	LEU	CA-C	6.17	1.61	1.52
1	A	225	ILE	CA-CB	6.01	1.62	1.54
1	A	326	ILE	CA-C	5.82	1.60	1.52
1	A	21	HIS	CG-ND1	-5.76	1.31	1.38
1	A	21	HIS	CD2-NE2	-5.52	1.31	1.37
1	A	207	THR	CA-CB	5.36	1.62	1.53
1	A	185	PHE	CA-C	5.33	1.58	1.52
1	A	293	ASN	CA-CB	-5.25	1.45	1.52
1	A	144	PHE	CA-CB	-5.14	1.44	1.53
1	A	297	VAL	CA-CB	5.10	1.61	1.54
1	A	293	ASN	CA-C	-5.06	1.47	1.53

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ASN	CA-CB-CG	14.90	127.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	ASP	CA-CB-CG	12.59	125.19	112.60
1	A	92	ASP	CA-C-O	-9.98	106.24	120.51
1	A	95	SER	N-CA-C	8.99	123.55	108.90
1	A	119	GLY	O-C-N	-8.96	113.90	122.86
1	A	316	ASN	CB-CG-ND2	8.88	129.72	116.40
1	A	197	THR	N-CA-CB	-8.78	97.06	109.97
1	A	91	LYS	CA-C-O	8.63	132.85	120.51
1	A	230	PHE	CA-CB-CG	8.60	122.40	113.80
1	A	42	ARG	CA-CB-CG	-8.56	96.99	114.10
1	A	115	PHE	O-C-N	-8.55	111.48	121.32
1	A	221	ASP	CA-CB-CG	8.47	121.07	112.60
1	A	26	ASN	N-CA-C	8.46	124.70	113.20
1	A	165	ASP	CA-CB-CG	8.43	121.03	112.60
1	A	200	GLN	OE1-CD-NE2	-8.27	114.33	122.60
1	A	336	MET	CB-CG-SD	-8.23	88.00	112.70
1	A	260	VAL	CG1-CB-CG2	-8.19	92.79	110.80
1	A	316	ASN	O-C-N	8.18	132.99	122.93
1	A	185	PHE	CA-CB-CG	7.98	121.78	113.80
1	A	130	THR	N-CA-CB	-7.96	98.52	110.07
1	A	185	PHE	O-C-N	-7.96	113.64	123.44
1	A	198	ASN	N-CA-C	7.96	120.96	111.33
1	A	316	ASN	OD1-CG-ND2	-7.92	114.68	122.60
1	A	185	PHE	N-CA-C	7.91	122.72	108.48
1	A	267	PHE	CA-CB-CG	7.84	121.64	113.80
1	A	218	LEU	CA-C-O	-7.81	111.92	120.36
1	A	136	LEU	N-CA-C	7.81	121.56	108.20
1	A	128	PHE	CA-CB-CG	7.80	121.60	113.80
1	A	241	THR	N-CA-C	-7.59	103.01	111.28
1	A	327	ASN	O-C-N	7.57	133.24	123.24
1	A	205	ARG	N-CA-C	7.56	121.77	109.59
1	A	329	ASP	N-CA-C	7.53	120.93	108.96
1	A	194	SER	O-C-N	-7.43	114.50	123.27
1	A	80	LYS	CA-CB-CG	7.22	128.53	114.10
1	A	70	ALA	O-C-N	-7.17	114.62	122.79
1	A	127	ASN	OD1-CG-ND2	-7.16	115.44	122.60
1	A	299	ALA	CA-C-O	-7.10	112.29	120.31
1	A	64	GLU	N-CA-C	-7.08	95.72	110.80
1	A	125	THR	CA-C-O	-7.08	113.84	121.56
1	A	161	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	A	327	ASN	CB-CA-C	-6.86	101.26	110.79
1	A	128	PHE	CA-C-O	-6.76	110.84	120.51
1	A	330	ASP	CA-CB-CG	6.72	119.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	GLN	OE1-CD-NE2	-6.71	115.89	122.60
1	A	169	GLN	CG-CD-NE2	6.71	126.47	116.40
1	A	195	ASP	CA-CB-CG	6.70	119.30	112.60
1	A	293	ASN	CB-CG-ND2	6.67	126.41	116.40
1	A	99	GLY	CA-C-O	-6.62	116.00	121.76
1	A	292	VAL	O-C-N	-6.62	115.92	123.07
1	A	234	THR	OG1-CB-CG2	6.57	122.43	109.30
1	A	189	GLY	O-C-N	-6.56	117.52	123.36
1	A	208	GLY	CA-C-O	6.53	126.93	121.05
1	A	223	ASN	CA-C-O	6.51	129.64	122.03
1	A	20	MET	CG-SD-CE	-6.50	86.60	100.90
1	A	129	MET	N-CA-C	6.47	124.59	110.80
1	A	169	GLN	N-CA-C	6.47	119.97	110.59
1	A	199	GLU	CA-C-N	6.47	131.67	120.68
1	A	199	GLU	C-N-CA	6.47	131.67	120.68
1	A	194	SER	CA-CB-OG	6.45	123.99	111.10
1	A	95	SER	CA-C-O	6.38	127.25	120.36
1	A	282	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	70	ALA	CA-C-O	-6.33	114.52	121.87
1	A	64	GLU	O-C-N	6.27	130.93	122.59
1	A	160	LYS	CA-CB-CG	6.24	126.59	114.10
1	A	59	GLY	N-CA-C	-6.21	101.39	110.90
1	A	326	ILE	O-C-N	-6.17	114.86	122.57
1	A	232	SER	O-C-N	-6.17	116.57	123.48
1	A	56	THR	CA-CB-OG1	-6.14	100.40	109.60
1	A	334	VAL	CA-C-O	-6.10	113.84	120.67
1	A	252	ASN	OD1-CG-ND2	-6.08	116.52	122.60
1	A	138	THR	OG1-CB-CG2	-6.07	97.17	109.30
1	A	69	LYS	O-C-N	-6.04	115.97	122.85
1	A	181	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	219	LYS	CA-CB-CG	6.02	126.13	114.10
1	A	121	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	228	ALA	O-C-N	-6.00	117.00	123.42
1	A	79	GLN	CG-CD-NE2	5.98	125.38	116.40
1	A	217	GLY	O-C-N	-5.95	118.07	123.36
1	A	123	ALA	N-CA-C	5.94	119.15	108.17
1	A	34	LYS	CA-CB-CG	5.91	125.91	114.10
1	A	338	TYR	N-CA-C	-5.90	100.67	110.17
1	A	223	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	12	ASP	N-CA-CB	-5.87	101.74	110.90
1	A	306	ASN	N-CA-C	5.85	120.71	112.93
1	A	78	GLN	CA-C-O	-5.84	112.15	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ASN	O-C-N	-5.82	114.85	122.59
1	A	126	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	56	THR	CA-CB-CG2	5.82	120.39	110.50
1	A	164	ARG	N-CA-C	5.80	123.16	110.80
1	A	172	ASP	CA-CB-CG	5.74	118.34	112.60
1	A	186	ALA	N-CA-C	5.74	118.00	108.99
1	A	225	ILE	CB-CA-C	5.72	120.20	111.68
1	A	64	GLU	CA-CB-CG	-5.68	102.73	114.10
1	A	79	GLN	OE1-CD-NE2	-5.68	116.92	122.60
1	A	121	ASP	N-CA-CB	-5.68	102.04	110.61
1	A	131	LYS	O-C-N	-5.67	115.05	122.59
1	A	129	MET	CA-C-N	5.66	128.13	120.44
1	A	129	MET	C-N-CA	5.66	128.13	120.44
1	A	15	GLY	N-CA-C	5.63	118.72	110.38
1	A	197	THR	CB-CA-C	5.61	119.25	109.65
1	A	214	TRP	CG-CD1-NE1	-5.61	102.91	110.20
1	A	46	LYS	CB-CG-CD	-5.60	98.42	111.30
1	A	66	ALA	N-CA-C	5.60	117.52	110.24
1	A	294	TYR	CA-CB-CG	5.59	123.97	113.90
1	A	95	SER	CA-CB-OG	5.56	122.22	111.10
1	A	262	GLN	CG-CD-NE2	-5.52	108.11	116.40
1	A	236	LYS	N-CA-C	5.52	119.05	111.54
1	A	320	SER	CA-CB-OG	5.51	122.12	111.10
1	A	128	PHE	O-C-N	-5.48	115.30	122.59
1	A	165	ASP	N-CA-CB	-5.48	102.43	110.26
1	A	307	MET	N-CA-CB	-5.48	101.48	110.52
1	A	316	ASN	N-CA-CB	5.43	117.94	109.85
1	A	68	ASN	N-CA-C	5.43	119.90	113.28
1	A	130	THR	CB-CA-C	5.42	119.47	110.90
1	A	308	SER	O-C-N	-5.41	117.20	122.99
1	A	187	ILE	CA-C-O	-5.40	115.38	121.75
1	A	171	GLY	CA-C-O	-5.39	116.89	122.28
1	A	69	LYS	CA-CB-CG	5.38	124.87	114.10
1	A	5	ASN	OD1-CG-ND2	-5.38	117.22	122.60
1	A	194	SER	CA-C-O	-5.36	114.42	120.32
1	A	183(A)	GLY	N-CA-C	-5.35	105.83	113.86
1	A	93	LEU	N-CA-C	5.34	122.17	110.80
1	A	275	TYR	O-C-N	-5.34	117.08	123.27
1	A	286	ILE	N-CA-CB	-5.33	105.39	112.26
1	A	126	ASP	CA-C-N	5.32	129.80	121.76
1	A	126	ASP	C-N-CA	5.32	129.80	121.76
1	A	48	GLU	CA-C-N	-5.31	113.83	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	GLU	C-N-CA	-5.31	113.83	121.42
1	A	189	GLY	CA-C-O	-5.30	116.70	121.47
1	A	197	THR	O-C-N	-5.30	116.43	122.89
1	A	179	THR	N-CA-CB	-5.28	101.94	110.81
1	A	258	GLU	CA-C-O	-5.28	114.94	121.11
1	A	13	VAL	CG1-CB-CG2	-5.28	99.19	110.80
1	A	21	HIS	O-C-N	-5.27	116.38	123.23
1	A	147	VAL	N-CA-C	5.23	120.21	109.34
1	A	178	LEU	N-CA-C	5.21	117.11	109.24
1	A	317	GLN	OE1-CD-NE2	-5.20	117.40	122.60
1	A	101	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	240	ILE	CA-CB-CG1	-5.19	101.58	110.40
1	A	265	PHE	N-CA-C	5.19	116.79	110.41
1	A	21	HIS	N-CA-CB	-5.17	101.83	110.83
1	A	311	VAL	CA-C-N	-5.17	114.56	122.62
1	A	311	VAL	C-N-CA	-5.17	114.56	122.62
1	A	35	ASP	O-C-N	-5.16	117.37	123.41
1	A	185	PHE	CB-CA-C	-5.16	101.03	109.80
1	A	201	ASN	CA-CB-CG	5.16	117.76	112.60
1	A	170	ASN	CB-CA-C	-5.15	101.78	110.43
1	A	317	GLN	O-C-N	-5.14	115.91	122.34
1	A	60	ARG	CA-CB-CG	-5.14	103.82	114.10
1	A	186	ALA	O-C-N	-5.12	117.55	123.33
1	A	141	ASN	CB-CG-ND2	5.11	124.07	116.40
1	A	316	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	118	PHE	N-CA-CB	-5.10	103.31	110.25
1	A	271	PRO	CA-C-O	-5.09	115.65	121.56
1	A	265	PHE	O-C-N	-5.09	116.44	122.65
1	A	46	LYS	CA-CB-CG	5.07	124.24	114.10
1	A	266	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	42	ARG	CG-CD-NE	-5.06	100.87	112.00
1	A	113	ASP	N-CA-C	-5.06	105.37	112.25
1	A	69	LYS	N-CA-C	5.05	117.37	110.55
1	A	224	ASN	OD1-CG-ND2	-5.05	117.55	122.60
1	A	219	LYS	CA-C-N	5.03	129.73	122.44
1	A	219	LYS	C-N-CA	5.03	129.73	122.44
1	A	308	SER	CA-CB-OG	5.03	121.16	111.10
1	A	78	GLN	CB-CA-C	-5.02	100.42	110.42
1	A	111	TRP	CE2-CD2-CE3	5.02	123.82	118.80
1	A	183(B)	SER	N-CA-C	-5.02	100.11	110.80
1	A	86	ALA	N-CA-C	-5.01	100.12	110.80
1	A	132	ARG	CD-NE-CZ	-5.01	117.39	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	MET	CB-CG-SD	-5.01	97.67	112.70
1	A	130	THR	O-C-N	-5.01	116.68	122.09
1	A	91	LYS	O-C-N	5.00	129.25	122.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	TYR	Sidechain
1	A	338	TYR	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	2602	0	2439	80	0
All	All	2602	0	2439	80	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 17.

All (80) 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:123:ALA:HA	1:A:130:THR:HG23	1.65	0.77
1:A:19:ALA:HA	1:A:39:SER:HB3	1.67	0.75
1:A:286:ILE:HG23	1:A:323:LYS:HB3	1.70	0.73
1:A:20:MET:HE2	1:A:310:PHE:HZ	1.58	0.69
1:A:24:SER:HB3	1:A:331:ILE:HA	1.76	0.68
1:A:136:LEU:HD23	1:A:158:GLN:HG3	1.76	0.67
1:A:250:PHE:H	1:A:250:PHE:HD1	1.40	0.67
1:A:123:ALA:HA	1:A:130:THR:CG2	2.27	0.63
1:A:162:GLU:HA	1:A:169:GLN:HG2	1.82	0.62
1:A:100:ARG:HG2	1:A:100:ARG:HH11	1.64	0.62
1:A:309:ALA:HA	1:A:336:MET:HA	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ALA:H	1:A:100:ARG:HB3	1.64	0.62
1:A:220:TYR:HE2	1:A:225:ILE:HG23	1.65	0.61
1:A:175:GLY:HA2	1:A:191:TYR:O	2.01	0.60
1:A:20:MET:HE2	1:A:310:PHE:CZ	2.35	0.60
1:A:227:LEU:HA	1:A:260:VAL:O	2.01	0.59
1:A:205:ARG:HD2	1:A:248:GLY:HA3	1.85	0.57
1:A:58:TYR:O	1:A:86:ALA:HA	2.04	0.57
1:A:18:LYS:HZ3	1:A:117:GLU:HG2	1.70	0.56
1:A:63:ALA:HA	1:A:81:THR:HA	1.87	0.56
1:A:62:GLU:OE1	1:A:82:ARG:HD3	2.06	0.55
1:A:115:PHE:HE1	1:A:260:VAL:CG2	2.19	0.55
1:A:173:GLY:HA3	1:A:194:SER:HA	1.88	0.55
1:A:231:TYR:OH	1:A:255:GLN:HG2	2.07	0.54
1:A:165:ASP:HB3	1:A:168:LYS:HG2	1.90	0.53
1:A:234:THR:O	1:A:253:LYS:HA	2.08	0.53
1:A:220:TYR:OH	1:A:222:ALA:HB3	2.07	0.53
1:A:240:ILE:HD11	1:A:291:LEU:HD11	1.91	0.52
1:A:19:ALA:CA	1:A:39:SER:HB3	2.38	0.52
1:A:262:GLN:NE2	1:A:272:SER:HB2	2.24	0.52
1:A:19:ALA:HA	1:A:39:SER:CB	2.40	0.52
1:A:216:THR:O	1:A:230:PHE:HB2	2.11	0.51
1:A:220:TYR:CZ	1:A:222:ALA:HB3	2.45	0.51
1:A:18:LYS:HG2	1:A:20:MET:HE3	1.91	0.50
1:A:169:GLN:OE1	1:A:197:THR:HG21	2.12	0.50
1:A:69:LYS:HG3	1:A:78:GLN:HG2	1.93	0.50
1:A:121(A):SER:HB3	1:A:256:ASN:HB3	1.92	0.50
1:A:225:ILE:HG13	1:A:226:TYR:N	2.25	0.50
1:A:241:THR:HG23	1:A:324:LEU:HD22	1.93	0.50
1:A:121(A):SER:OG	1:A:276:VAL:HG13	2.14	0.48
1:A:280:GLY:O	1:A:288:ASP:HB3	2.13	0.48
1:A:294:TYR:CD1	1:A:314:LYS:HG3	2.49	0.48
1:A:60:ARG:HG2	1:A:61:TRP:N	2.28	0.47
1:A:101:ASN:HB3	1:A:136:LEU:HD12	1.97	0.47
1:A:20:MET:SD	1:A:117:GLU:OE2	2.73	0.47
1:A:40:TYR:CE1	1:A:42:ARG:NH1	2.82	0.47
1:A:303:PHE:HD2	1:A:308:SER:HA	1.80	0.46
1:A:4:TYR:O	1:A:10:LYS:HA	2.16	0.46
1:A:4:TYR:CE1	1:A:6:LYS:HD3	2.50	0.46
1:A:177:SER:HB3	1:A:190:ALA:HB2	1.97	0.46
1:A:84:ALA:O	1:A:100:ARG:N	2.49	0.46
1:A:16:LYS:NZ	1:A:42:ARG:NH2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLN:OE1	1:A:281:LYS:HD2	2.15	0.45
1:A:140:ARG:HA	1:A:153:LEU:O	2.16	0.45
1:A:98:TYR:HA	1:A:136:LEU:O	2.17	0.45
1:A:59:GLY:HA2	1:A:86:ALA:HA	1.99	0.44
1:A:60:ARG:HH11	1:A:60:ARG:HD2	1.53	0.44
1:A:100:ARG:HH11	1:A:100:ARG:CG	2.31	0.44
1:A:278:SER:O	1:A:291:LEU:N	2.48	0.43
1:A:11:LEU:HD23	1:A:11:LEU:HA	1.90	0.43
1:A:128:PHE:CD1	1:A:128:PHE:N	2.85	0.43
1:A:326:ILE:HG22	1:A:327:ASN:H	1.84	0.43
1:A:165:ASP:O	1:A:169:GLN:HG3	2.18	0.43
1:A:277:LEU:HA	1:A:292:VAL:O	2.18	0.43
1:A:111:TRP:CE2	1:A:219:LYS:HG2	2.54	0.42
1:A:139:TYR:CE2	1:A:141:ASN:HB2	2.54	0.42
1:A:238:THR:HA	1:A:239:PRO:HD2	1.69	0.42
1:A:240:ILE:HD12	1:A:324:LEU:HD13	2.01	0.42
1:A:130:THR:OG1	1:A:237:MET:HE2	2.19	0.42
1:A:293:ASN:ND2	1:A:317:GLN:HB3	2.34	0.42
1:A:205:ARG:CD	1:A:248:GLY:HA3	2.49	0.42
1:A:240:ILE:HD13	1:A:240:ILE:HA	1.63	0.42
1:A:115:PHE:HB2	1:A:118:PHE:O	2.20	0.41
1:A:139:TYR:O	1:A:154:THR:HA	2.20	0.41
1:A:262:GLN:HE21	1:A:272:SER:HB2	1.86	0.41
1:A:21:HIS:CE1	1:A:36:GLY:HA2	2.57	0.40
1:A:129:MET:HB2	1:A:129:MET:HE3	1.61	0.40
1:A:216:THR:O	1:A:230:PHE:HA	2.21	0.40
1:A:57:GLY:HA2	1:A:87:GLY:O	2.21	0.40
1:A:127:ASN:O	1:A:130:THR:HB	2.22	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	A	328/330 (99%)	269 (82%)	45 (14%)	14 (4%)	2	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	LEU
1	A	144	PHE
1	A	164	ARG
1	A	2	GLU
1	A	128	PHE
1	A	284	GLU
1	A	326	ILE
1	A	34	LYS
1	A	51	ILE
1	A	24	SER
1	A	103	GLY
1	A	250	PHE
1	A	285	GLY
1	A	147	VAL

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	267/267 (100%)	214 (80%)	53 (20%)	1	7

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	16	LYS
1	A	23	MET
1	A	24	SER
1	A	35	ASP
1	A	38	GLN
1	A	39	SER

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Mol	Chain	Res	Type
1	A	50	GLN
1	A	52	ASN
1	A	56	THR
1	A	69	LYS
1	A	79	GLN
1	A	80	LYS
1	A	82	ARG
1	A	100	ARG
1	A	105	LEU
1	A	111	TRP
1	A	117	GLU
1	A	125	THR
1	A	128	PHE
1	A	129	MET
1	A	130	THR
1	A	132	ARG
1	A	142	THR
1	A	152	ASN
1	A	163	ASN
1	A	194	SER
1	A	197	THR
1	A	198	ASN
1	A	204	SER
1	A	207	THR
1	A	209	LYS
1	A	210	ARG
1	A	216	THR
1	A	225	ILE
1	A	232	SER
1	A	240	ILE
1	A	241	THR
1	A	250	PHE
1	A	252	ASN
1	A	256	ASN
1	A	272	SER
1	A	273	LEU
1	A	281	LYS
1	A	283	ILE
1	A	284	GLU
1	A	288	ASP
1	A	291	LEU
1	A	316	ASN

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Mol	Chain	Res	Type
1	A	317	GLN
1	A	325	ASN
1	A	327	ASN
1	A	328	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	21	HIS
1	A	38	GLN
1	A	127	ASN
1	A	203	GLN
1	A	293	ASN
1	A	339	GLN

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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.