



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:32 PM GMT

PDB ID : 1PHO
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

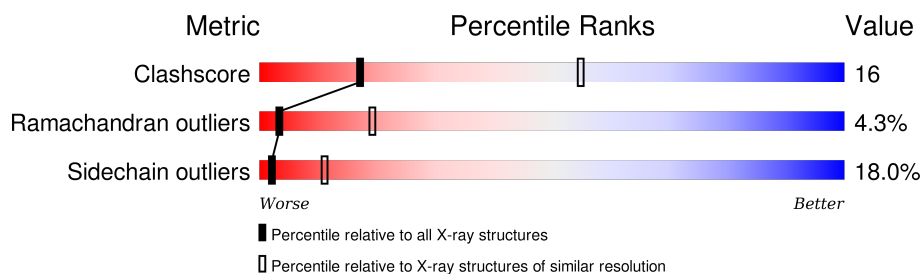
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	330	 48% 38% 11%

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.

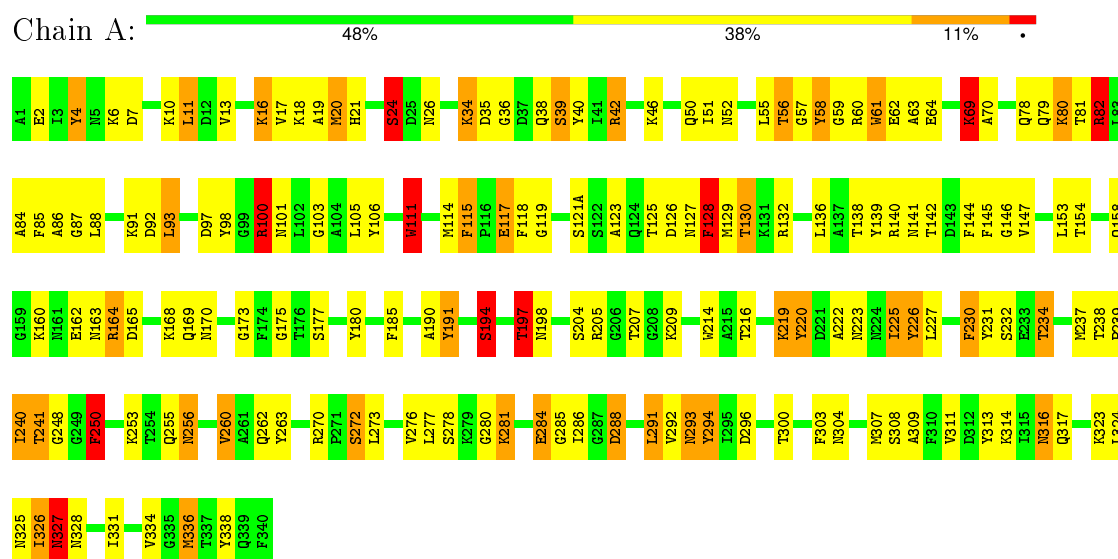
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	330	2602	1631	437	527	7	203	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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 will therefore be incomplete.

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.90 Å 119.90 Å 51.90 Å 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 i

5.1 Standard geometry i

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	1.07	1/2654 (0.0%)	2.02	82/3575 (2.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	THR	CA-CB	5.50	1.67	1.53

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	VAL	CG1-CB-CG2	-11.32	92.79	110.90
1	A	58	TYR	CB-CG-CD1	-10.21	114.87	121.00
1	A	214	TRP	CD1-CG-CD2	9.65	114.02	106.30
1	A	82	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	A	91	LYS	CA-C-N	-8.97	97.46	117.20
1	A	180	TYR	CB-CG-CD1	-8.70	115.78	121.00
1	A	4	TYR	CB-CG-CD1	-8.68	115.79	121.00
1	A	191	TYR	CB-CG-CD1	-8.52	115.89	121.00
1	A	20	MET	CG-SD-CE	-8.50	86.60	100.20
1	A	336	MET	CB-CG-SD	-8.13	88.00	112.40
1	A	58	TYR	CB-CG-CD2	7.67	125.60	121.00
1	A	128	PHE	CA-C-N	7.50	133.69	117.20
1	A	42	ARG	CA-CB-CG	-7.46	96.99	113.40
1	A	214	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	82	ARG	NE-CZ-NH1	7.40	124.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	VAL	CG1-CB-CG2	-7.32	99.19	110.90
1	A	61	TRP	CD1-CG-CD2	7.28	112.12	106.30
1	A	214	TRP	CG-CD1-NE1	-7.19	102.91	110.10
1	A	313	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	A	223	ASN	CA-C-N	-7.04	101.72	117.20
1	A	197	THR	N-CA-CB	-6.97	97.06	110.30
1	A	336	MET	CG-SD-CE	6.91	111.26	100.20
1	A	80	LYS	CA-CB-CG	6.88	128.53	113.40
1	A	100	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	327	ASN	CA-C-N	-6.61	102.65	117.20
1	A	92	ASP	CA-C-O	-6.60	106.24	120.10
1	A	327	ASN	O-C-N	6.58	133.24	122.70
1	A	111	TRP	NE1-CE2-CD2	6.57	113.86	107.30
1	A	146	GLY	CA-C-N	-6.54	102.81	117.20
1	A	61	TRP	CE2-CD2-CG	-6.53	102.08	107.30
1	A	316	ASN	O-C-N	6.43	132.99	122.70
1	A	304	ASN	CA-CB-CG	6.41	127.50	113.40
1	A	194	SER	CA-C-N	6.27	131.00	117.20
1	A	130	THR	N-CA-CB	-6.20	98.52	110.30
1	A	70	ALA	CA-C-N	6.17	130.78	117.20
1	A	111	TRP	NE1-CE2-CZ2	-6.12	123.67	130.40
1	A	55	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	91	LYS	CA-C-O	6.07	132.85	120.10
1	A	114	MET	CA-CB-CG	6.06	123.60	113.30
1	A	4	TYR	CB-CG-CD2	6.00	124.60	121.00
1	A	160	LYS	CA-CB-CG	5.99	126.59	113.40
1	A	106	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	92	ASP	CA-C-N	5.95	130.30	117.20
1	A	88	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	111	TRP	CE2-CD2-CG	-5.83	102.63	107.30
1	A	219	LYS	CA-CB-CG	5.79	126.13	113.40
1	A	296	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	126	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	56	THR	CA-CB-CG2	5.70	120.39	112.40
1	A	34	LYS	CA-CB-CG	5.69	125.91	113.40
1	A	164	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	64	GLU	N-CA-C	-5.66	95.72	111.00
1	A	185	PHE	O-C-N	-5.66	113.64	122.70
1	A	145	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	A	237	MET	CA-CB-CG	5.58	122.79	113.30
1	A	138	THR	OG1-CB-CG2	-5.58	97.17	110.00
1	A	316	ASN	CA-C-N	-5.57	104.95	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	TYR	CA-CB-CG	5.56	123.97	113.40
1	A	226	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	296	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	263	TYR	CB-CG-CD2	-5.51	117.70	121.00
1	A	119	GLY	O-C-N	-5.47	113.90	123.20
1	A	93	LEU	CA-CB-CG	5.43	127.79	115.30
1	A	316	ASN	CB-CG-ND2	5.42	129.72	116.70
1	A	311	VAL	CG1-CB-CG2	-5.42	102.23	110.90
1	A	234	THR	OG1-CB-CG2	5.40	122.43	110.00
1	A	97	ASP	CA-CB-CG	5.36	125.19	113.40
1	A	334	VAL	CA-C-N	5.27	126.73	116.20
1	A	69	LYS	CA-CB-CG	5.21	124.87	113.40
1	A	42	ARG	CG-CD-NE	-5.21	100.87	111.80
1	A	85	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	A	64	GLU	O-C-N	5.14	130.93	122.70
1	A	194	SER	O-C-N	-5.13	114.50	122.70
1	A	26	ASN	N-CA-C	5.08	124.70	111.00
1	A	46	LYS	CB-CG-CD	-5.07	98.42	111.60
1	A	307	MET	N-CA-CB	-5.07	101.48	110.60
1	A	115	PHE	O-C-N	-5.06	111.48	121.10
1	A	270	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	17	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	A	70	ALA	O-C-N	-5.05	114.62	122.70
1	A	129	MET	N-CA-C	5.03	124.59	111.00
1	A	70	ALA	CB-CA-C	-5.02	102.58	110.10

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	75	0
All	All	2602	0	2439	75	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 16.

All (75) 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: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:HD1	1:A:250:PHE:H	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:309:ALA:HA	1:A:336:MET:HA	1.79	0.62
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.64	0.62
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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:18:LYS:HZ1	1:A:117:GLU:HG2	1.77	0.49
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:255:GLN:OE1	1:A:281:LYS:HD2	2.15	0.45
1:A:16:LYS:NZ	1:A:42:ARG:NH2	2.64	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:HD2	1:A:60:ARG:HH11	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:N	1:A:128:PHE:CD1	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:139:TYR:CE2	1:A:141:ASN:HB2	2.54	0.42
1:A:111:TRP:CE2	1:A:219:LYS:HG2	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: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:HA	1:A:240:ILE:HD13	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:216:THR:O	1:A:230:PHE:HA	2.21	0.40
1:A:21:HIS:CE1	1:A:36:GLY:HA2	2.57	0.40
1:A:127:ASN:O	1:A:130:THR:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:GLY:HA2	1:A:87:GLY:O	2.21	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%)	3	19

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 [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	267/267 (100%)	219 (82%)	48 (18%)	2 11

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	11	LEU
1	A	16	LYS
1	A	24	SER
1	A	35	ASP
1	A	38	GLN
1	A	39	SER
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	132	ARG
1	A	142	THR
1	A	163	ASN
1	A	170	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	225	ILE
1	A	230	PHE
1	A	232	SER
1	A	240	ILE

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Mol	Chain	Res	Type
1	A	241	THR
1	A	250	PHE
1	A	256	ASN
1	A	272	SER
1	A	273	LEU
1	A	281	LYS
1	A	284	GLU
1	A	288	ASP
1	A	291	LEU
1	A	293	ASN
1	A	316	ASN
1	A	325	ASN
1	A	327	ASN
1	A	328	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	HIS
1	A	38	GLN
1	A	170	ASN
1	A	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.