WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 01:49 AM EDT

PDB ID	:	3GEY
Title	:	Crystal structure of human poly(ADP-ribose) polymerase 15, catalytic fragment in complex with an inhibitor Pj34
Authors	:	Karlberg, T.; Siponen, M.I.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Kotenyova, T.; Moche, M.; Nordlund, P.; Nyman, T.; Persson, C.; Sagemark, J.; Schutz, P.; Thorsell, A.G.; Tresaugues, L.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Schuler, H.; Structural Genomics Consortium (SGC)
Deposited on	:	2009-02-26
Resolution	:	2.20 Å(reported)

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

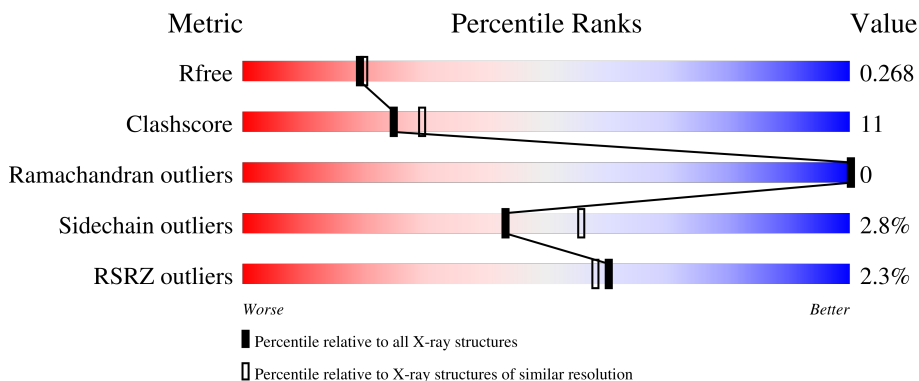|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

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 2.20 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		11
Ramachandran outliers		0
Sidechain outliers		2.8%
RSRZ outliers		2.3%

Worse .... *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	221	3% / 67% 17% • 15%
1	B	221	3% / 70% 15% 14%

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Mol	Chain	Length	Quality of chain
1	C	221	% 67% 21% • 12%
1	D	221	% 69% 17% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	P34	A	701	-	-	X	-

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6295 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 Poly [ADP-ribose] polymerase 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1531	972	265	287	7			
1	B	190	Total	C	N	O	S	0	0	0
			1552	985	270	290	7			
1	C	195	Total	C	N	O	S	0	0	0
			1564	992	270	295	7			
1	D	195	Total	C	N	O	S	0	0	0
			1577	999	275	296	7			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	MET	-	expression tag	UNP Q460N3
A	437	HIS	-	expression tag	UNP Q460N3
A	438	HIS	-	expression tag	UNP Q460N3
A	439	HIS	-	expression tag	UNP Q460N3
A	440	HIS	-	expression tag	UNP Q460N3
A	441	HIS	-	expression tag	UNP Q460N3
A	442	HIS	-	expression tag	UNP Q460N3
A	443	SER	-	expression tag	UNP Q460N3
A	444	SER	-	expression tag	UNP Q460N3
A	445	GLY	-	expression tag	UNP Q460N3
A	446	VAL	-	expression tag	UNP Q460N3
A	447	ASP	-	expression tag	UNP Q460N3
A	448	LEU	-	expression tag	UNP Q460N3
A	449	GLY	-	expression tag	UNP Q460N3
A	450	THR	-	expression tag	UNP Q460N3
A	451	GLU	-	expression tag	UNP Q460N3
A	452	ASN	-	expression tag	UNP Q460N3
A	453	LEU	-	expression tag	UNP Q460N3
A	454	TYR	-	expression tag	UNP Q460N3
A	455	PHE	-	expression tag	UNP Q460N3
A	456	GLN	-	expression tag	UNP Q460N3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	457	SER	-	expression tag	UNP Q460N3
A	458	MET	-	expression tag	UNP Q460N3
B	436	MET	-	expression tag	UNP Q460N3
B	437	HIS	-	expression tag	UNP Q460N3
B	438	HIS	-	expression tag	UNP Q460N3
B	439	HIS	-	expression tag	UNP Q460N3
B	440	HIS	-	expression tag	UNP Q460N3
B	441	HIS	-	expression tag	UNP Q460N3
B	442	HIS	-	expression tag	UNP Q460N3
B	443	SER	-	expression tag	UNP Q460N3
B	444	SER	-	expression tag	UNP Q460N3
B	445	GLY	-	expression tag	UNP Q460N3
B	446	VAL	-	expression tag	UNP Q460N3
B	447	ASP	-	expression tag	UNP Q460N3
B	448	LEU	-	expression tag	UNP Q460N3
B	449	GLY	-	expression tag	UNP Q460N3
B	450	THR	-	expression tag	UNP Q460N3
B	451	GLU	-	expression tag	UNP Q460N3
B	452	ASN	-	expression tag	UNP Q460N3
B	453	LEU	-	expression tag	UNP Q460N3
B	454	TYR	-	expression tag	UNP Q460N3
B	455	PHE	-	expression tag	UNP Q460N3
B	456	GLN	-	expression tag	UNP Q460N3
B	457	SER	-	expression tag	UNP Q460N3
B	458	MET	-	expression tag	UNP Q460N3
C	436	MET	-	expression tag	UNP Q460N3
C	437	HIS	-	expression tag	UNP Q460N3
C	438	HIS	-	expression tag	UNP Q460N3
C	439	HIS	-	expression tag	UNP Q460N3
C	440	HIS	-	expression tag	UNP Q460N3
C	441	HIS	-	expression tag	UNP Q460N3
C	442	HIS	-	expression tag	UNP Q460N3
C	443	SER	-	expression tag	UNP Q460N3
C	444	SER	-	expression tag	UNP Q460N3
C	445	GLY	-	expression tag	UNP Q460N3
C	446	VAL	-	expression tag	UNP Q460N3
C	447	ASP	-	expression tag	UNP Q460N3
C	448	LEU	-	expression tag	UNP Q460N3
C	449	GLY	-	expression tag	UNP Q460N3
C	450	THR	-	expression tag	UNP Q460N3
C	451	GLU	-	expression tag	UNP Q460N3
C	452	ASN	-	expression tag	UNP Q460N3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	453	LEU	-	expression tag	UNP Q460N3
C	454	TYR	-	expression tag	UNP Q460N3
C	455	PHE	-	expression tag	UNP Q460N3
C	456	GLN	-	expression tag	UNP Q460N3
C	457	SER	-	expression tag	UNP Q460N3
C	458	MET	-	expression tag	UNP Q460N3
D	436	MET	-	expression tag	UNP Q460N3
D	437	HIS	-	expression tag	UNP Q460N3
D	438	HIS	-	expression tag	UNP Q460N3
D	439	HIS	-	expression tag	UNP Q460N3
D	440	HIS	-	expression tag	UNP Q460N3
D	441	HIS	-	expression tag	UNP Q460N3
D	442	HIS	-	expression tag	UNP Q460N3
D	443	SER	-	expression tag	UNP Q460N3
D	444	SER	-	expression tag	UNP Q460N3
D	445	GLY	-	expression tag	UNP Q460N3
D	446	VAL	-	expression tag	UNP Q460N3
D	447	ASP	-	expression tag	UNP Q460N3
D	448	LEU	-	expression tag	UNP Q460N3
D	449	GLY	-	expression tag	UNP Q460N3
D	450	THR	-	expression tag	UNP Q460N3
D	451	GLU	-	expression tag	UNP Q460N3
D	452	ASN	-	expression tag	UNP Q460N3
D	453	LEU	-	expression tag	UNP Q460N3
D	454	TYR	-	expression tag	UNP Q460N3
D	455	PHE	-	expression tag	UNP Q460N3
D	456	GLN	-	expression tag	UNP Q460N3
D	457	SER	-	expression tag	UNP Q460N3
D	458	MET	-	expression tag	UNP Q460N3

- Molecule 2 is N 2 ,N 2 -DIMETHYL-N 1 -(6-OXO-5,6-DIHYDROPHENANTHRIDIN-2-YL)GLYCINAMIDE (three-letter code: P34) (formula: $C_{17}H_{17}N_3O_2$).
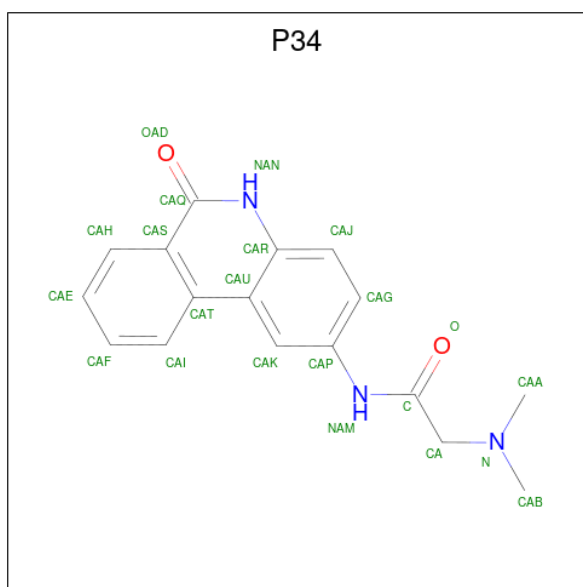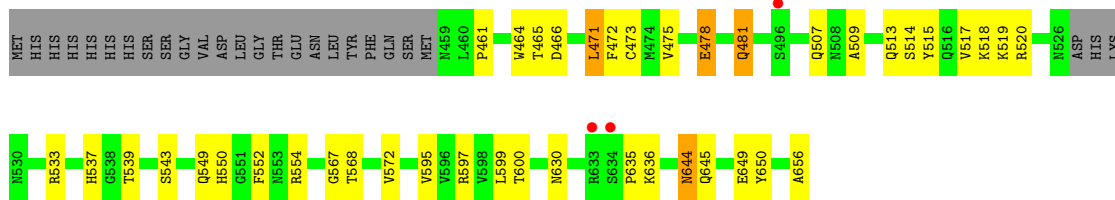
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 22	C 17	N 3	O 2	0	0
2	B	1	Total 22	C 17	N 3	O 2	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	7	Total 7	O 7	0	0
3	C	6	Total 6	O 6	0	0
3	D	11	Total 11	O 11	0	0

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 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.

• Molecule 1: Poly [ADP-ribose] polymerase 15

• Molecule 1: Poly [ADP-ribose] polymerase 15

• Molecule 1: Poly [ADP-ribose] polymerase 15

• Molecule 1: Poly [ADP-ribose] polymerase 15

MET HIS HIS HIS HIS HIS SER SER GLY VAL ASP LEU GLY THR GLU ASN LEU TYR PHE GLN SER MET N459 L460 P461 W464 T465 D466 L471 F472 C473 M474 V475 E478 Q481 S496 Q507 N508 A509 Q513 S514 Y515 Q516 V517 K518 K519 R520 N526 ASP HIS LYS

N530 R533 H537 G538 T539 S543 Q549 H550 G551 F552 N553 R554 G567 T568 V572 V595 V596 R597 V598 L599 T600 N630 R633 S634 P635 K636 N644 Q645 E649 Y650 A656

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	45.08Å 137.63Å 68.05Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	24.19 – 2.20 24.19 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (24.19-2.20) 97.5 (24.19-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	5.52 (at 2.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.212 , 0.270 0.213 , 0.268	Depositor DCC
R_{free} test set	1996 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 20.7	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.407 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6295	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: P34

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	0.28	0/1572	0.44	0/2128
1	B	0.30	0/1595	0.46	0/2161
1	C	0.31	0/1606	0.47	0/2178
1	D	0.32	0/1619	0.45	0/2193
All	All	0.30	0/6392	0.46	0/8660

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	1531	0	1468	36	0
1	B	1552	0	1488	28	0
1	C	1564	0	1490	31	0
1	D	1577	0	1516	33	0
2	A	22	0	17	10	0
2	B	22	0	17	6	0
3	A	3	0	0	0	0
3	B	7	0	0	0	0
3	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11	0	0	1	0
All	All	6295	0	5996	133	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 11.

All (133) 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:D:481:GLN:HE21	1:D:481:GLN:HA	0.96	1.09
2:B:701:P34:HAM	2:B:701:P34:HAA1	1.19	1.06
1:A:571:ALA:HB2	2:A:701:P34:HAH	1.41	1.01
1:A:514:SER:HB3	1:A:644:ASN:HD22	1.27	0.97
1:D:481:GLN:HA	1:D:481:GLN:NE2	1.79	0.96
1:A:597:ARG:HG2	1:A:597:ARG:HH21	1.28	0.96
1:A:597:ARG:HH21	1:A:597:ARG:CG	1.88	0.86
1:B:463:HIS:HD2	1:B:464:TRP:HD1	1.21	0.86
1:B:463:HIS:CD2	1:B:464:TRP:HD1	1.94	0.85
1:A:538:GLY:O	2:A:701:P34:HAJ	1.82	0.79
2:B:701:P34:HAM	2:B:701:P34:CAA	2.00	0.75
1:A:514:SER:HB3	1:A:644:ASN:ND2	2.00	0.75
1:B:509:ALA:O	1:B:513:GLN:HG3	1.86	0.74
1:D:481:GLN:HE21	1:D:481:GLN:CA	1.85	0.72
1:C:539:THR:HG21	1:C:543:SER:HB2	1.70	0.71
1:A:525:LYS:HE3	1:A:526:ASN:OD1	1.91	0.71
2:B:701:P34:HAA1	2:B:701:P34:NAM	1.99	0.70
1:A:622:THR:HB	1:D:549:GLN:HG3	1.74	0.69
1:B:463:HIS:CD2	1:B:464:TRP:CD1	2.79	0.69
2:A:701:P34:O	2:A:701:P34:HAG	1.93	0.68
1:A:597:ARG:HG2	1:A:597:ARG:NH2	2.07	0.68
2:B:701:P34:O	2:B:701:P34:HAG	1.92	0.67
1:A:465:THR:HG23	1:A:505:ARG:NH2	2.11	0.66
1:A:517:VAL:HG21	1:D:517:VAL:HG21	1.80	0.64
1:D:514:SER:HB3	1:D:644:ASN:HD22	1.62	0.64
1:B:552:PHE:HB3	1:B:568:THR:HG21	1.82	0.62
1:A:607:ARG:O	1:A:610:LEU:HG	2.01	0.61
1:A:630:ASN:ND2	1:A:636:LYS:HG2	2.16	0.60
1:A:588:ASN:HB3	1:A:590:ARG:HH11	1.65	0.60
1:C:561:ALA:HB2	1:D:478:GLU:OE2	2.02	0.60
1:C:513:GLN:O	1:C:517:VAL:HG23	2.02	0.59
1:A:630:ASN:HD21	1:A:636:LYS:HG2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:MET:HG2	1:B:473:CYS:SG	2.43	0.59
1:B:537:HIS:CD2	1:B:539:THR:HG23	2.37	0.59
1:C:501:GLU:HG2	1:C:653:THR:HB	1.85	0.59
1:D:519:LYS:HG3	1:D:599:LEU:HD21	1.83	0.58
1:A:552:PHE:CE2	1:A:648:PRO:HG3	2.37	0.58
1:B:588:ASN:HB3	1:B:590:ARG:HH11	1.69	0.58
2:A:701:P34:HAA1	2:A:701:P34:NAM	2.18	0.57
1:C:539:THR:CG2	1:C:543:SER:HB2	2.34	0.57
1:A:644:ASN:OD1	1:A:644:ASN:N	2.37	0.57
1:D:644:ASN:N	1:D:644:ASN:OD1	2.38	0.57
1:C:552:PHE:HB3	1:C:568:THR:HG21	1.87	0.56
1:A:467:MET:O	1:A:470:GLN:HG3	2.05	0.56
1:A:465:THR:HG23	1:A:505:ARG:HH21	1.71	0.56
1:B:617:ASN:HB3	1:B:620:ASN:OD1	2.04	0.56
1:B:622:THR:HB	1:C:549:GLN:HG3	1.88	0.55
1:C:509:ALA:O	1:C:513:GLN:HG3	2.05	0.55
1:D:630:ASN:ND2	1:D:636:LYS:HG2	2.21	0.55
1:A:552:PHE:HB3	1:A:568:THR:HG21	1.89	0.55
1:A:460:LEU:HD22	1:A:460:LEU:N	2.22	0.54
1:B:461:PRO:HG3	1:B:512:TRP:CZ2	2.42	0.53
1:A:509:ALA:O	1:A:513:GLN:HG3	2.09	0.53
1:B:533:ARG:HD2	1:B:600:THR:HG21	1.91	0.53
1:A:636:LYS:HG3	1:A:637:LEU:HD23	1.92	0.52
1:C:597:ARG:HE	1:C:649:GLU:CD	2.13	0.52
1:D:630:ASN:HD21	1:D:636:LYS:HG2	1.75	0.51
1:C:501:GLU:HG3	1:C:502:LYS:N	2.25	0.51
1:C:620:ASN:OD1	1:C:623:ASP:HB2	2.10	0.51
1:B:517:VAL:HG21	1:C:517:VAL:HG21	1.92	0.50
1:C:539:THR:HG22	1:C:540:ASP:N	2.27	0.50
1:B:460:LEU:HD12	1:B:460:LEU:N	2.27	0.50
2:B:701:P34:O	2:B:701:P34:CAG	2.60	0.50
1:C:491:PHE:CD1	1:C:593:MET:HE3	2.47	0.50
1:B:490:LYS:HG2	1:B:493:ARG:HH22	1.77	0.50
1:A:525:LYS:NZ	1:A:626:ASP:OD1	2.46	0.49
1:D:465:THR:HG21	1:D:475:VAL:HG11	1.94	0.49
1:C:574:ALA:HB1	1:C:593:MET:HE3	1.94	0.49
1:A:538:GLY:O	2:A:701:P34:CAJ	2.59	0.49
1:B:619:HIS:C	1:B:620:ASN:ND2	2.66	0.48
1:D:471:LEU:HB3	3:D:803:HOH:O	2.13	0.48
1:A:597:ARG:CG	1:A:597:ARG:NH2	2.59	0.48
1:D:518:LYS:HB2	1:D:518:LYS:HE2	1.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:ASN:HB3	1:A:637:LEU:HD21	1.95	0.48
1:A:571:ALA:CB	2:A:701:P34:HAH	2.28	0.48
1:B:467:MET:HG3	1:B:507:GLN:NE2	2.28	0.48
1:C:491:PHE:HD1	1:C:593:MET:HE3	1.79	0.48
1:D:518:LYS:HE2	1:D:644:ASN:HB2	1.96	0.47
1:C:479:PRO:HA	1:C:484:TYR:CD2	2.49	0.47
1:A:615:PRO:HB3	1:A:621:PRO:HA	1.97	0.47
1:A:539:THR:OG1	1:A:543:SER:HB2	2.15	0.47
1:B:619:HIS:C	1:B:620:ASN:HD22	2.18	0.46
1:B:597:ARG:HE	1:B:649:GLU:CD	2.18	0.46
1:D:572:VAL:HG21	1:D:635:PRO:O	2.15	0.46
1:C:547:VAL:HG11	1:C:594:TYR:CZ	2.50	0.46
1:B:637:LEU:C	1:B:637:LEU:HD12	2.35	0.46
1:C:605:LYS:HE3	1:C:630:ASN:O	2.15	0.46
1:D:515:TYR:CE1	1:D:599:LEU:HG	2.51	0.46
1:D:514:SER:HB3	1:D:644:ASN:ND2	2.29	0.46
1:C:547:VAL:HG11	1:C:594:TYR:CE2	2.52	0.45
1:B:467:MET:O	1:B:470:GLN:HG3	2.17	0.45
1:C:547:VAL:CG1	1:C:594:TYR:CZ	3.00	0.45
2:A:701:P34:O	2:A:701:P34:CAG	2.61	0.45
1:B:472:PHE:HA	1:B:507:GLN:O	2.17	0.45
1:D:533:ARG:HD2	1:D:600:THR:HG21	1.99	0.44
1:A:461:PRO:HB2	1:A:464:TRP:CD1	2.52	0.44
1:D:539:THR:OG1	1:D:543:SER:HB2	2.18	0.44
1:A:467:MET:O	1:A:470:GLN:CG	2.66	0.44
1:C:512:TRP:CZ2	1:C:516:GLN:NE2	2.86	0.44
1:D:552:PHE:HB3	1:D:568:THR:HG21	1.99	0.44
1:B:620:ASN:ND2	1:B:620:ASN:N	2.66	0.43
1:C:609:GLY:HA3	1:D:656:ALA:O	2.18	0.43
1:D:537:HIS:CD2	1:D:552:PHE:HE1	2.36	0.43
1:A:533:ARG:HD2	1:A:600:THR:HG21	2.00	0.43
1:A:471:LEU:HD13	1:A:510:PHE:CZ	2.53	0.43
1:D:461:PRO:HG2	1:D:464:TRP:CE2	2.54	0.43
1:D:599:LEU:HB2	1:D:645:GLN:HG2	2.00	0.43
1:B:461:PRO:CG	1:B:512:TRP:CZ2	3.02	0.43
1:D:595:VAL:HB	1:D:650:TYR:HB2	2.01	0.43
1:C:474:MET:HE2	1:C:504:GLU:OE1	2.19	0.42
1:D:465:THR:CG2	1:D:475:VAL:HG11	2.48	0.42
1:B:517:VAL:O	1:B:521:GLN:HG3	2.19	0.42
1:C:515:TYR:CE1	1:C:599:LEU:HG	2.54	0.42
1:A:569:TYR:HD1	1:A:637:LEU:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:TYR:O	1:B:518:LYS:HB3	2.20	0.42
1:C:634:SER:N	1:C:635:PRO:HD3	2.34	0.42
1:D:472:PHE:CE2	1:D:549:GLN:NE2	2.88	0.42
1:A:538:GLY:H	2:A:701:P34:HAN	1.67	0.42
1:D:597:ARG:HD2	1:D:649:GLU:OE2	2.20	0.42
1:B:460:LEU:N	1:B:460:LEU:CD1	2.83	0.41
1:C:584:LYS:HA	1:C:585:PRO:HD3	1.91	0.41
2:A:701:P34:HAA1	2:A:701:P34:HAM	1.83	0.41
1:B:471:LEU:HD13	1:B:510:PHE:CZ	2.56	0.41
2:A:701:P34:HAK	2:A:701:P34:HAI	1.75	0.41
1:D:554:ARG:HB2	1:D:567:GLY:HA2	2.02	0.41
1:C:566:LYS:HD2	1:C:611:VAL:HG12	2.03	0.41
1:C:525:LYS:HB3	1:C:525:LYS:HE3	1.80	0.41
1:D:472:PHE:HA	1:D:507:GLN:O	2.20	0.41
1:D:509:ALA:O	1:D:513:GLN:HG3	2.20	0.41
1:C:472:PHE:CZ	1:C:548:ASN:HB3	2.56	0.40
1:C:604:THR:HG21	1:C:614:PRO:HG2	2.03	0.40
2:B:701:P34:HAI	2:B:701:P34:HAK	1.80	0.40
1:D:549:GLN:HB2	1:D:550:HIS:CD2	2.56	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	182/221 (82%)	178 (98%)	4 (2%)	0	100	100
1	B	186/221 (84%)	177 (95%)	9 (5%)	0	100	100
1	C	191/221 (86%)	187 (98%)	4 (2%)	0	100	100
1	D	191/221 (86%)	186 (97%)	5 (3%)	0	100	100
All	All	750/884 (85%)	728 (97%)	22 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	170/198 (86%)	165 (97%)	5 (3%)	42	54
1	B	173/198 (87%)	172 (99%)	1 (1%)	86	93
1	C	171/198 (86%)	165 (96%)	6 (4%)	36	46
1	D	174/198 (88%)	167 (96%)	7 (4%)	31	40
All	All	688/792 (87%)	669 (97%)	19 (3%)	43	56

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	462	GLU
1	A	466	ASP
1	A	470	GLN
1	A	597	ARG
1	A	644	ASN
1	B	620	ASN
1	C	501	GLU
1	C	581	THR
1	C	593	MET
1	C	607	ARG
1	C	633	ARG
1	C	643	ASP
1	D	466	ASP
1	D	471	LEU
1	D	473	CYS
1	D	478	GLU
1	D	481	GLN
1	D	520	ARG
1	D	644	ASN

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

Mol	Chain	Res	Type
1	B	463	HIS
1	B	468	ASN
1	D	481	GLN
1	D	530	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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	P34	A	701	-	23,24,24	1.62	5 (21%)	30,34,34	2.02	4 (13%)
2	P34	B	701	-	23,24,24	1.66	3 (13%)	30,34,34	1.95	3 (10%)

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	P34	A	701	-	-	0/8/8/8	0/3/3/3

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WORLDWIDE
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PROTEIN DATA BANK

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	P34	B	701	-	-	0/8/8/8	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	P34	CAQ-NAN	4.26	1.40	1.33
2	A	701	P34	CAQ-NAN	3.79	1.39	1.33
2	B	701	P34	CAP-NAM	-3.59	1.34	1.41
2	B	701	P34	CAR-NAN	3.56	1.41	1.35
2	A	701	P34	CAP-NAM	-3.53	1.34	1.41
2	A	701	P34	CAR-NAN	2.77	1.39	1.35
2	A	701	P34	CAT-CAU	-2.06	1.38	1.45
2	A	701	P34	CAT-CAS	-2.04	1.38	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	P34	CAU-CAR-NAN	-6.93	119.84	123.60
2	B	701	P34	CAS-CAQ-NAN	-6.35	119.97	124.40
2	B	701	P34	CAU-CAR-NAN	-6.24	120.21	123.60
2	A	701	P34	CAS-CAQ-NAN	-6.04	120.19	124.40
2	A	701	P34	CAB-N-CA	-2.40	106.43	110.38
2	B	701	P34	CAP-NAM-C	-2.17	123.70	127.50
2	A	701	P34	CAK-CAU-CAR	2.14	120.51	118.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	P34	10	0
2	B	701	P34	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand P34 A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand P34 B 701

Bond lengths

Bond angles

Torsions

Rings
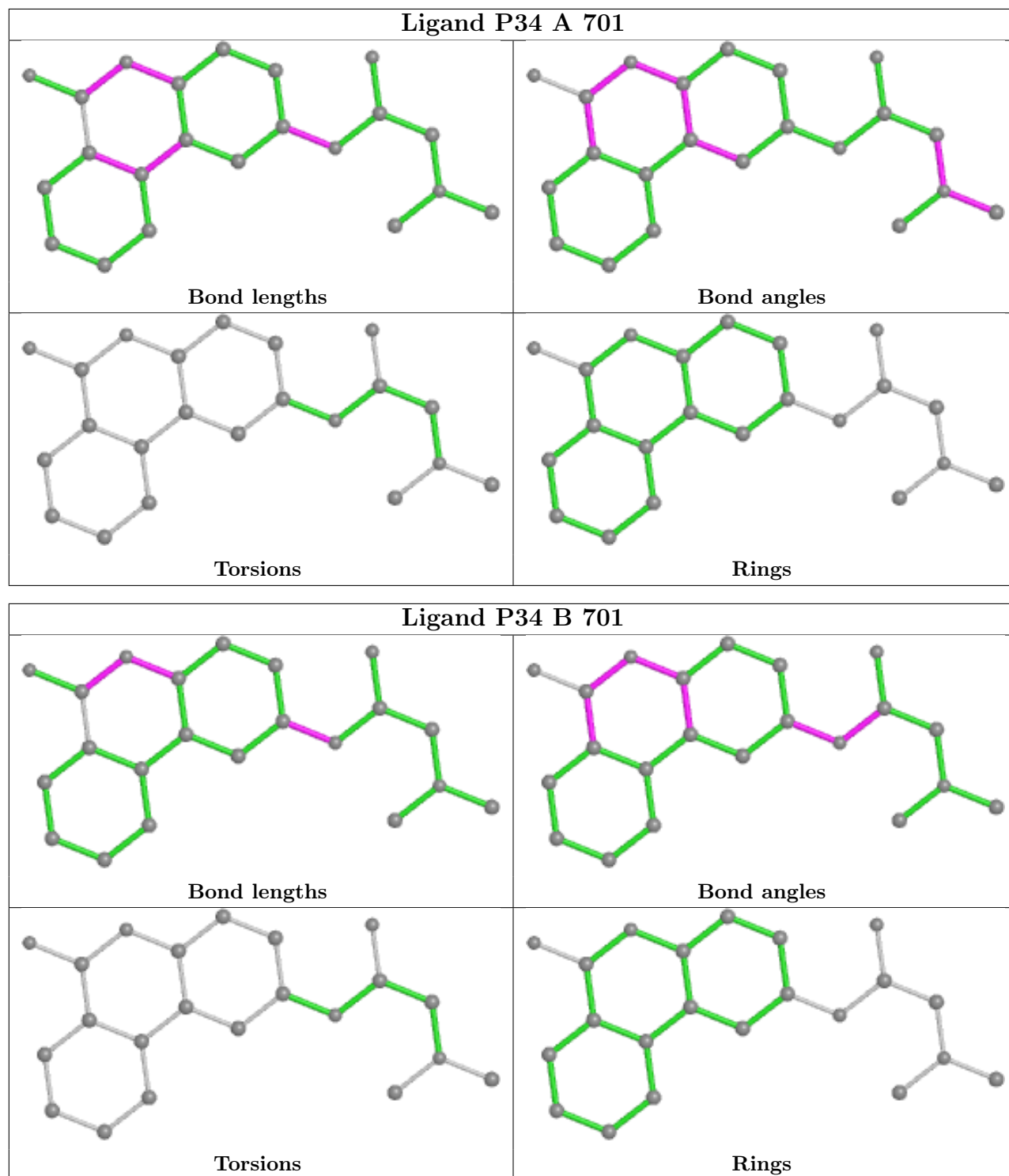
5.7 Other polymers ⓘ

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	188/221 (85%)	0.39	6 (3%)	47	45	20, 30, 50, 63	0
1	B	190/221 (85%)	0.47	6 (3%)	47	45	21, 32, 52, 74	0
1	C	195/221 (88%)	0.16	3 (1%)	73	72	15, 25, 39, 59	0
1	D	195/221 (88%)	0.20	3 (1%)	73	72	17, 25, 38, 68	0
All	All	768/884 (86%)	0.30	18 (2%)	60	58	15, 28, 49, 74	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	622	THR	3.5
1	B	622	THR	3.2
1	C	656	ALA	2.9
1	A	617	ASN	2.9
1	A	621	PRO	2.8
1	B	460	LEU	2.7
1	D	633	ARG	2.6
1	C	496	SER	2.4
1	C	469	HIS	2.4
1	D	496	SER	2.4
1	A	644	ASN	2.3
1	B	618	PRO	2.3
1	B	623	ASP	2.2
1	B	480	GLY	2.2
1	B	590	ARG	2.1
1	D	634	SER	2.1
1	A	620	ASN	2.1
1	A	618	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

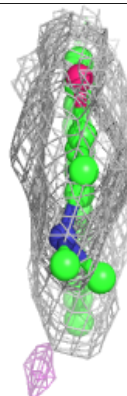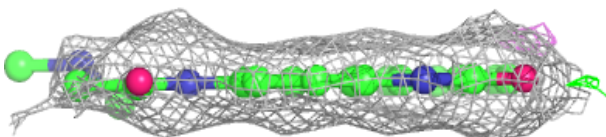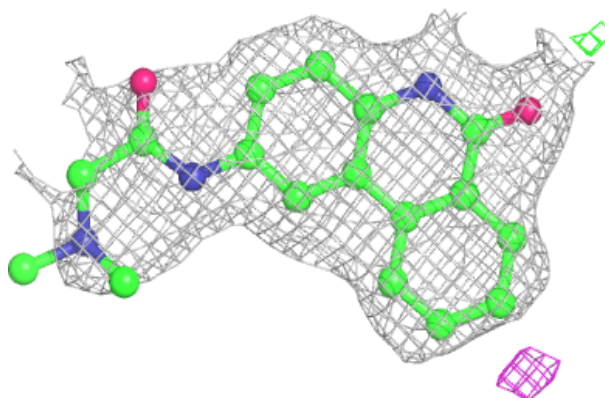| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	P34	A	701	22/22	0.85	0.22	26,34,53,70	0
2	P34	B	701	22/22	0.88	0.19	30,38,57,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P34 A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
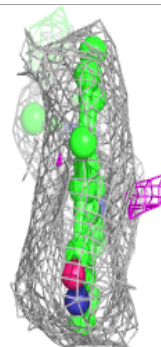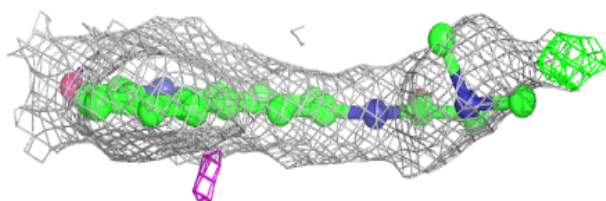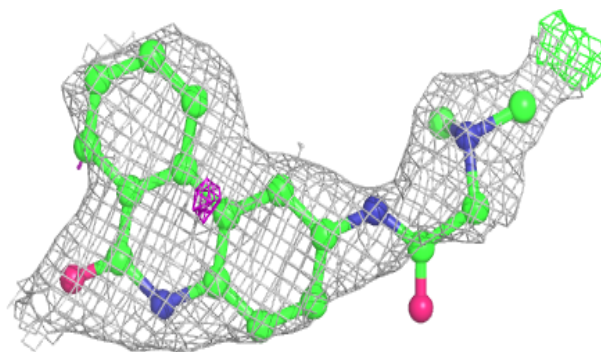
Electron density around P34 B 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.