



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:45 PM UTC

PDB ID : 3L2K / pdb_00003l2k
Title : Structure of phenazine antibiotic biosynthesis protein with substrate
Authors : Bera, A.K.; Atanasova, V.; Parsons, J.F.
Deposited on : 2009-12-15
Resolution : 2.80 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

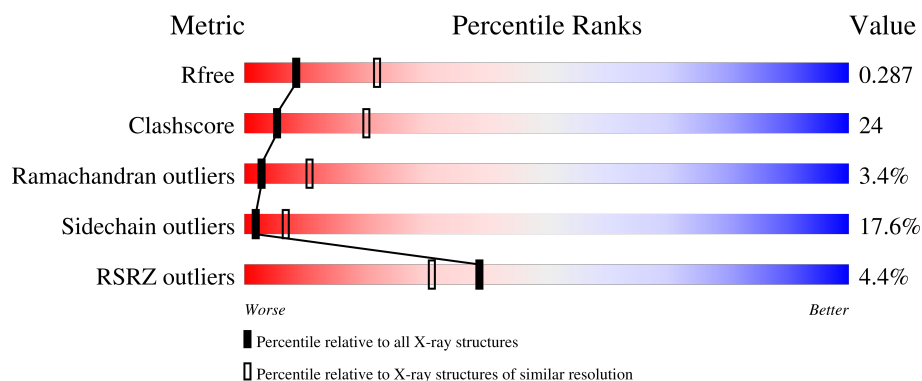
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	366	3% 45% 35% 12% 5%
1	B	366	5% 46% 34% 14%

2 Entry composition [i](#)

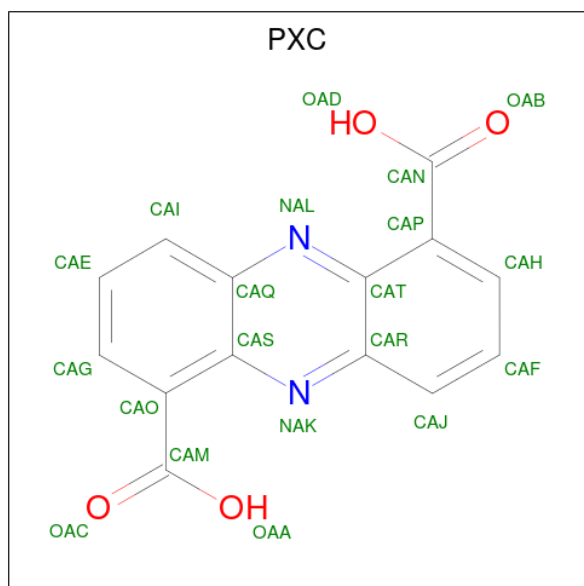
There are 3 unique types of molecules in this entry. The entry contains 5594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 EhpF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2769	1758	478	524	9			
1	B	352	Total	C	N	O	S	0	0	0
			2769	1758	478	524	9			

- Molecule 2 is phenazine-1,6-dicarboxylic acid (CCD ID: PXC) (formula: $C_{14}H_8N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	14	2	4		
2	B	1	Total	C	N	O	0	0
			20	14	2	4		

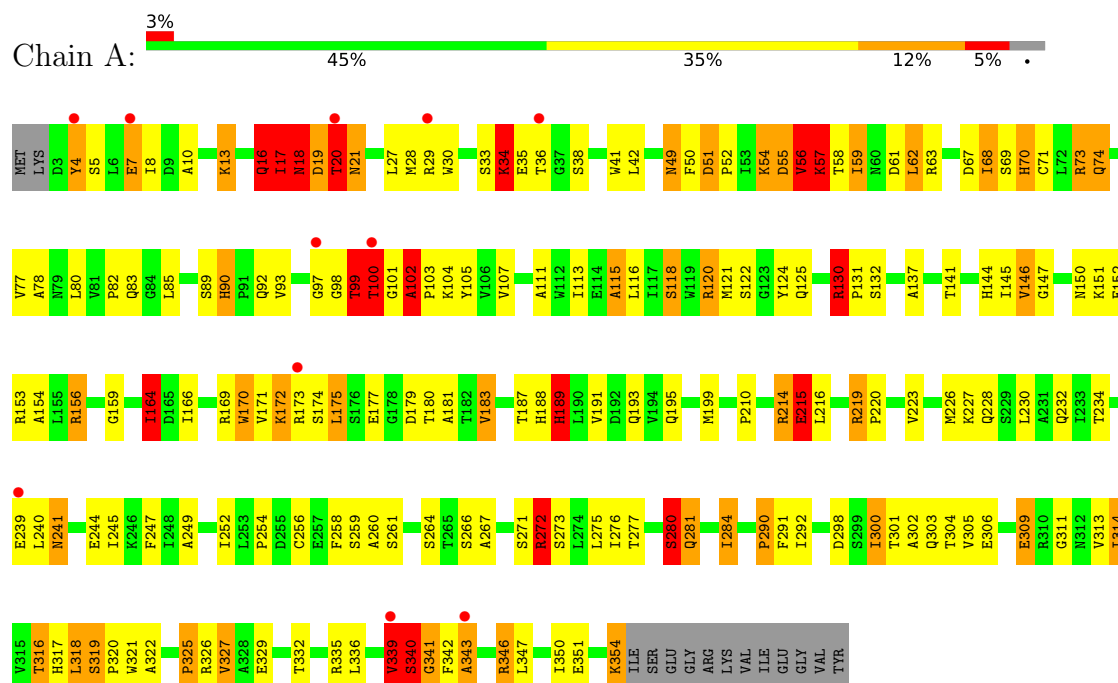
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0
3	B	7	Total 7	O 7	0	0

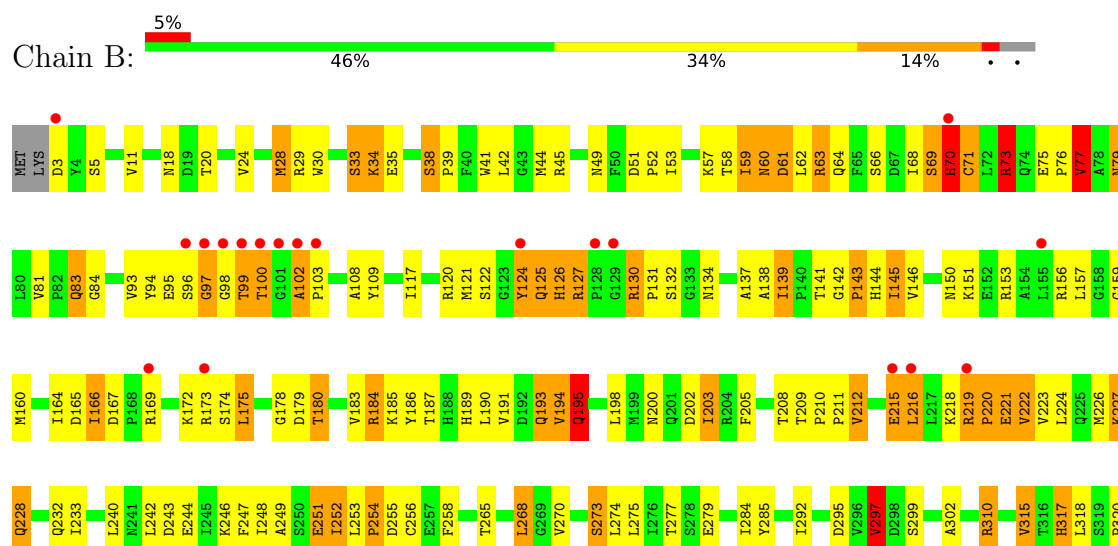
3 Residue-property plots

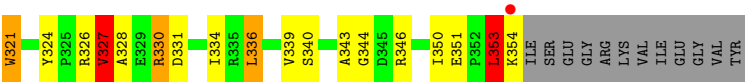
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: EhpfF



• Molecule 1: EhpfF





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	193.13Å 193.13Å 193.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.78 – 2.80 26.78 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.78-2.80) 99.7 (26.78-2.81)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.288 0.213 , 0.287	Depositor DCC
R_{free} test set	1495 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5594	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.69	28/2834 (1.0%)	1.72	52/3857 (1.3%)
1	B	1.64	31/2834 (1.1%)	1.69	51/3857 (1.3%)
All	All	1.67	59/5668 (1.0%)	1.71	103/7714 (1.3%)

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	7
1	B	0	2
All	All	0	9

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ILE	CA-CB	-9.22	1.43	1.54
1	B	49	ASN	CA-C	8.49	1.63	1.53
1	A	259	SER	CA-C	-8.18	1.42	1.52
1	A	122	SER	C-O	7.84	1.34	1.23
1	B	143	PRO	CA-C	7.67	1.60	1.52
1	B	99	THR	CA-C	7.64	1.62	1.52
1	A	113	ILE	CA-CB	-7.63	1.45	1.54
1	B	83	GLN	CA-C	-7.49	1.42	1.52
1	B	3	ASP	N-CA	7.41	1.60	1.46
1	A	102	ALA	CA-C	7.19	1.58	1.52
1	B	96	SER	CA-C	-6.91	1.44	1.52
1	A	292	ILE	CA-CB	-6.79	1.46	1.54
1	B	343	ALA	CA-CB	-6.51	1.42	1.53
1	A	115	ALA	CA-CB	-6.50	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	LYS	CA-C	6.28	1.60	1.52
1	B	75	GLU	CA-C	6.28	1.60	1.53
1	B	44	MET	SD-CE	6.27	1.95	1.79
1	B	28	MET	C-O	6.23	1.31	1.24
1	B	100	THR	N-CA	6.19	1.54	1.46
1	B	41	TRP	C-O	-6.08	1.17	1.24
1	B	126	HIS	N-CA	-6.05	1.38	1.46
1	A	164	ILE	CA-C	-6.04	1.46	1.53
1	A	261	SER	CA-C	-5.83	1.45	1.52
1	B	143	PRO	C-O	5.81	1.30	1.23
1	B	336	LEU	N-CA	5.79	1.52	1.45
1	B	354	LYS	C-O	5.67	1.34	1.23
1	A	57	LYS	CA-C	5.66	1.58	1.52
1	B	99	THR	N-CA	5.64	1.53	1.46
1	B	219	ARG	CZ-NH1	5.63	1.40	1.32
1	A	154	ALA	CA-CB	-5.61	1.44	1.53
1	A	99	THR	CA-CB	5.58	1.61	1.53
1	A	105	TYR	N-CA	5.53	1.53	1.46
1	A	137	ALA	CA-CB	-5.52	1.45	1.53
1	B	327	VAL	CA-CB	-5.50	1.47	1.54
1	A	260	ALA	CA-CB	-5.48	1.43	1.53
1	B	254	PRO	N-CA	-5.45	1.41	1.47
1	A	276	ILE	CA-CB	-5.42	1.47	1.53
1	A	245	ILE	N-CA	-5.40	1.40	1.46
1	A	107	VAL	N-CA	-5.38	1.40	1.46
1	A	256	CYS	N-CA	-5.37	1.39	1.46
1	A	316	THR	CA-CB	-5.35	1.45	1.53
1	A	340	SER	CA-C	5.32	1.59	1.52
1	B	145	ILE	CA-CB	-5.31	1.47	1.54
1	A	327	VAL	C-O	5.29	1.29	1.24
1	B	164	ILE	C-O	-5.28	1.18	1.23
1	B	35	GLU	CA-CB	-5.26	1.45	1.53
1	B	61	ASP	CA-C	5.25	1.60	1.52
1	A	170	TRP	N-CA	-5.24	1.39	1.46
1	B	11	VAL	CA-CB	-5.19	1.48	1.54
1	B	344	GLY	C-O	-5.16	1.18	1.24
1	A	183	VAL	CA-CB	5.15	1.60	1.54
1	A	219	ARG	CA-C	-5.15	1.46	1.52
1	B	143	PRO	N-CD	5.13	1.54	1.47
1	B	315	VAL	CA-CB	-5.12	1.48	1.54
1	A	4	TYR	N-CA	5.12	1.51	1.46
1	A	34	LYS	N-CA	5.09	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	TRP	CA-C	5.09	1.59	1.52
1	B	143	PRO	N-CA	-5.08	1.42	1.47
1	B	44	MET	N-CA	-5.04	1.39	1.46

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	PRO	CA-N-CD	-10.58	96.69	111.50
1	B	142	GLY	CA-C-N	-10.19	109.18	121.00
1	B	142	GLY	C-N-CA	-10.19	109.18	121.00
1	B	96	SER	N-CA-C	-9.15	95.33	108.96
1	B	336	LEU	CA-C-N	-9.00	110.76	119.76
1	B	336	LEU	C-N-CA	-9.00	110.76	119.76
1	A	343	ALA	N-CA-C	8.60	121.45	108.46
1	A	36	THR	N-CA-C	8.60	122.27	111.69
1	A	16	GLN	N-CA-C	8.37	124.17	113.88
1	B	143	PRO	CA-N-CD	-8.36	100.29	112.00
1	A	102	ALA	CA-C-N	8.35	147.03	127.00
1	A	102	ALA	C-N-CA	8.35	147.03	127.00
1	A	239	GLU	N-CA-C	-7.95	100.66	111.87
1	B	134	ASN	N-CA-C	7.80	121.54	110.23
1	B	18	ASN	N-CA-C	7.74	122.08	111.39
1	B	222	VAL	N-CA-C	-7.60	103.45	110.82
1	B	124	TYR	N-CA-C	7.59	122.44	112.72
1	B	44	MET	N-CA-C	-7.59	103.28	112.54
1	A	90	HIS	CA-C-N	7.20	127.16	120.03
1	A	90	HIS	C-N-CA	7.20	127.16	120.03
1	A	150	ASN	N-CA-C	7.19	119.19	111.36
1	A	340	SER	N-CA-C	7.16	126.06	110.80
1	A	102	ALA	C-N-CD	-7.04	105.12	120.60
1	B	34	LYS	CA-C-N	-7.02	109.78	121.92
1	B	34	LYS	C-N-CA	-7.02	109.78	121.92
1	B	227	LYS	N-CA-C	-7.00	103.67	111.71
1	B	183	VAL	N-CA-C	-6.82	103.88	110.42
1	B	254	PRO	CA-C-N	-6.79	112.69	122.67
1	B	254	PRO	C-N-CA	-6.79	112.69	122.67
1	A	188	HIS	CA-C-O	6.60	127.97	120.90
1	B	79	ASN	N-CA-C	6.60	120.59	112.54
1	A	309	GLU	N-CA-C	6.53	120.26	110.14
1	B	194	VAL	N-CA-C	6.51	116.54	110.42
1	B	75	GLU	CA-C-N	-6.41	112.55	119.98
1	B	75	GLU	C-N-CA	-6.41	112.55	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	GLN	CB-CA-C	6.40	121.13	109.99
1	A	280	SER	CA-C-N	-6.37	112.36	122.29
1	A	280	SER	C-N-CA	-6.37	112.36	122.29
1	B	70	HIS	N-CA-C	-6.32	98.53	108.63
1	B	252	ILE	N-CA-C	6.29	116.34	110.42
1	B	242	LEU	N-CA-C	6.29	117.93	111.14
1	A	159	GLY	N-CA-C	-6.27	101.36	111.59
1	A	71	CYS	N-CA-C	6.25	118.18	111.36
1	A	99	THR	CB-CA-C	6.22	119.12	110.16
1	A	59	ILE	CB-CA-C	-6.21	102.54	112.16
1	B	297	VAL	N-CA-CB	-6.20	101.28	111.44
1	B	353	LEU	N-CA-C	6.16	123.93	110.80
1	A	223	VAL	CB-CA-C	-6.11	104.15	111.97
1	B	321	TRP	N-CA-C	6.11	120.47	112.89
1	A	339	VAL	N-CA-CB	6.09	117.81	110.31
1	B	193	GLN	N-CA-C	-6.07	104.78	111.82
1	A	258	PHE	N-CA-C	6.03	119.03	109.50
1	B	127	ARG	N-CA-C	5.98	116.48	109.60
1	B	274	LEU	N-CA-C	-5.93	101.50	110.28
1	B	219	ARG	CA-C-N	5.92	127.24	119.84
1	B	219	ARG	C-N-CA	5.92	127.24	119.84
1	A	118	SER	N-CA-CB	5.86	119.36	110.28
1	B	117	ILE	N-CA-C	-5.82	103.77	111.05
1	B	326	ARG	N-CA-C	5.79	119.56	111.74
1	A	214	ARG	N-CA-C	-5.78	104.90	111.14
1	A	339	VAL	CA-C-N	5.77	132.55	121.54
1	A	339	VAL	C-N-CA	5.77	132.55	121.54
1	A	351	GLU	CA-C-N	5.75	127.02	119.84
1	A	351	GLU	C-N-CA	5.75	127.02	119.84
1	B	255	ASP	N-CA-C	5.73	120.11	109.56
1	A	339	VAL	O-C-N	5.72	128.91	122.67
1	B	38	SER	N-CA-C	-5.70	102.46	109.65
1	A	132	SER	N-CA-C	5.69	117.83	109.24
1	A	271	SER	CA-C-N	-5.69	113.88	122.81
1	A	271	SER	C-N-CA	-5.69	113.88	122.81
1	B	150	ASN	N-CA-C	5.63	117.41	111.28
1	B	63	ARG	N-CA-C	-5.61	106.13	112.87
1	B	336	LEU	N-CA-C	5.59	119.22	109.82
1	A	189	HIS	N-CA-C	-5.59	105.72	112.54
1	B	268	LEU	CB-CA-C	-5.58	103.65	111.80
1	B	159	GLY	N-CA-C	-5.57	103.12	111.19
1	B	81	VAL	CB-CA-C	-5.52	104.81	110.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	GLU	N-CA-C	-5.45	105.25	112.34
1	A	80	LEU	N-CA-C	-5.44	106.69	113.38
1	A	244	GLU	N-CA-C	-5.33	105.37	111.07
1	B	73	ARG	N-CA-C	-5.33	104.37	111.24
1	A	120	ARG	NE-CZ-NH1	-5.32	116.18	121.50
1	A	93	VAL	CB-CA-C	-5.30	104.25	111.15
1	B	339	VAL	CB-CA-C	-5.26	102.66	111.29
1	B	59	ILE	CB-CA-C	-5.25	102.68	111.29
1	A	30	TRP	N-CA-C	-5.24	105.47	111.07
1	B	324	TYR	CA-C-N	-5.24	114.34	119.99
1	B	324	TYR	C-N-CA	-5.24	114.34	119.99
1	A	179	ASP	N-CA-C	5.22	117.21	108.23
1	A	111	ALA	N-CA-C	-5.20	105.51	111.07
1	A	327	VAL	N-CA-C	5.16	115.66	108.84
1	A	130	ARG	CG-CD-NE	5.16	123.35	112.00
1	A	322	ALA	CA-C-N	-5.16	115.50	122.77
1	A	322	ALA	C-N-CA	-5.16	115.50	122.77
1	A	215	GLU	N-CA-C	5.14	117.28	111.11
1	B	3	ASP	N-CA-C	5.13	125.37	111.00
1	A	346	ARG	CB-CA-C	-5.13	100.10	109.54
1	A	272	ARG	CG-CD-NE	-5.12	100.74	112.00
1	A	120	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	B	243	ASP	N-CA-C	-5.08	105.82	111.36
1	B	93	VAL	CB-CA-C	-5.06	104.05	110.98
1	A	146	VAL	N-CA-CB	5.05	116.46	110.55
1	A	276	ILE	CB-CA-C	-5.03	104.87	111.25

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	THR	Peptide
1	A	102	ALA	Peptide
1	A	17	ILE	Peptide
1	A	19	ASP	Peptide
1	A	325	PRO	Peptide
1	A	339	VAL	Peptide
1	A	99	THR	Peptide
1	B	70	HIS	Peptide
1	B	97	GLY	Peptide

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	2769	0	2737	148	0
1	B	2769	0	2737	128	0
2	A	20	0	6	2	0
2	B	20	0	6	3	0
3	A	9	0	0	0	0
3	B	7	0	0	0	0
All	All	5594	0	5486	265	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 24.

All (265) 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:B:184:ARG:HG3	1:B:184:ARG:HH11	1.13	1.12
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.09	1.12
1:A:4:TYR:O	1:A:8:ILE:HD12	1.57	1.05
1:B:73:ARG:HH12	1:B:102:ALA:HB1	1.15	1.05
1:B:73:ARG:NH1	1:B:102:ALA:HB1	1.70	1.04
1:A:16:GLN:HE21	1:A:16:GLN:N	1.55	1.04
1:B:102:ALA:HB3	1:B:103:PRO:HA	1.41	1.03
1:B:191:VAL:HG13	1:B:216:LEU:HD23	1.36	1.02
1:B:228:GLN:HA	1:B:228:GLN:HE21	1.22	1.02
1:A:193:GLN:HE21	1:B:169:ARG:HH11	1.07	0.97
1:B:228:GLN:HA	1:B:228:GLN:NE2	1.80	0.96
1:A:193:GLN:HE21	1:B:169:ARG:NH1	1.64	0.96
1:B:228:GLN:HE21	1:B:228:GLN:CA	1.77	0.95
1:A:341:GLY:HA3	1:A:342:PHE:HB2	1.49	0.93
1:A:340:SER:HA	1:A:341:GLY:O	1.69	0.92
1:A:169:ARG:NH1	1:B:193:GLN:HE21	1.66	0.92
1:B:130:ARG:HG2	1:B:130:ARG:NH1	1.79	0.91
1:A:169:ARG:HH11	1:B:193:GLN:HE21	0.97	0.91
1:A:74:GLN:HA	1:A:74:GLN:HE21	1.34	0.91
1:B:191:VAL:HG13	1:B:216:LEU:CD2	2.01	0.89
1:B:195:GLN:HG3	1:B:219:ARG:HH11	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ASN:C	1:A:241:ASN:OD1	2.16	0.88
1:B:102:ALA:CB	1:B:103:PRO:HA	2.02	0.88
1:A:16:GLN:C	1:A:18:ASN:H	1.83	0.86
1:B:130:ARG:HH11	1:B:130:ARG:CG	1.89	0.85
1:A:73:ARG:HG3	1:A:73:ARG:HH11	1.41	0.85
1:A:341:GLY:HA3	1:A:342:PHE:CB	2.04	0.85
1:A:341:GLY:CA	1:A:342:PHE:HB2	2.08	0.83
1:A:16:GLN:HE21	1:A:16:GLN:H	1.23	0.82
1:B:153:ARG:HH21	2:B:400:PXC:HAJ	1.45	0.81
1:A:28:MET:HE3	1:A:56:VAL:HG11	1.61	0.81
1:B:253:LEU:O	1:B:253:LEU:HD12	1.81	0.80
1:A:193:GLN:NE2	1:B:169:ARG:HH11	1.79	0.80
1:B:73:ARG:HH12	1:B:102:ALA:CB	1.92	0.80
1:A:169:ARG:HH11	1:B:193:GLN:NE2	1.79	0.79
1:B:143:PRO:HD2	1:B:144:HIS:CD2	2.16	0.79
1:B:68:ILE:O	1:B:71:CYS:HB3	1.82	0.79
1:A:226:MET:HG2	1:A:230:LEU:HD12	1.65	0.77
1:A:16:GLN:H	1:A:16:GLN:NE2	1.83	0.77
1:B:228:GLN:HE21	1:B:228:GLN:C	1.92	0.76
1:B:102:ALA:HB3	1:B:103:PRO:CA	2.16	0.75
1:B:124:TYR:HA	1:B:127:ARG:HG2	1.66	0.75
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.50	0.74
1:A:241:ASN:OD1	1:A:241:ASN:O	2.06	0.74
1:A:193:GLN:NE2	1:B:169:ARG:NH1	2.35	0.74
1:B:95:GLU:HG3	1:B:143:PRO:HB2	1.71	0.73
1:B:184:ARG:HH11	1:B:184:ARG:CG	1.95	0.72
1:A:63:ARG:NH2	1:A:302:ALA:O	2.23	0.72
1:A:49:ASN:HD22	1:A:49:ASN:C	1.98	0.71
1:A:56:VAL:HG12	1:A:56:VAL:O	1.87	0.71
1:B:195:GLN:HG3	1:B:219:ARG:NH1	2.05	0.70
1:A:68:ILE:HG12	1:A:68:ILE:O	1.91	0.70
1:A:290:PRO:HD2	1:A:291:PHE:H	1.57	0.70
1:B:184:ARG:HG3	1:B:184:ARG:NH1	1.94	0.69
1:A:298:ASP:OD2	1:A:301:THR:HG23	1.93	0.68
1:B:221:GLU:CD	1:B:221:GLU:H	2.01	0.67
1:B:131:PRO:O	1:B:132:SER:HB3	1.93	0.67
1:A:191:VAL:HG13	1:A:216:LEU:HD23	1.78	0.66
1:A:226:MET:HG2	1:A:230:LEU:CD1	2.25	0.66
1:A:266:SER:OG	1:A:327:VAL:HG21	1.96	0.65
1:A:4:TYR:C	1:A:8:ILE:HD12	2.21	0.65
1:A:267:ALA:HB1	1:A:317:HIS:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ARG:NH2	2:A:400:PXC:HAJ	2.12	0.64
1:B:102:ALA:CB	1:B:103:PRO:CA	2.72	0.64
1:A:180:THR:HG23	1:A:181:ALA:N	2.11	0.63
1:A:290:PRO:HD2	1:A:291:PHE:N	2.11	0.63
1:A:317:HIS:NE2	1:A:319:SER:HB3	2.13	0.63
1:B:63:ARG:NH1	1:B:295:ASP:OD2	2.31	0.63
1:B:130:ARG:NH1	1:B:131:PRO:O	2.31	0.63
1:A:273:SER:HA	1:A:284:ILE:O	1.99	0.63
1:B:124:TYR:O	1:B:130:ARG:HD3	1.98	0.63
1:B:297:VAL:HG13	1:B:302:ALA:HA	1.81	0.62
1:B:336:LEU:HB2	1:B:346:ARG:HB3	1.81	0.61
1:B:121:MET:HE1	1:B:156:ARG:HD2	1.81	0.61
1:B:210:PRO:HD2	1:B:211:PRO:HD3	1.81	0.61
1:A:28:MET:HE1	1:A:62:LEU:CD2	2.29	0.61
1:A:16:GLN:N	1:A:16:GLN:NE2	2.35	0.61
1:A:74:GLN:HA	1:A:74:GLN:NE2	2.11	0.61
1:A:191:VAL:HG21	1:A:215:GLU:HG3	1.83	0.61
1:B:178:GLY:O	1:B:180:THR:HG22	2.01	0.60
1:B:228:GLN:NE2	1:B:228:GLN:O	2.34	0.60
1:B:317:HIS:C	1:B:317:HIS:CD2	2.80	0.60
1:A:16:GLN:C	1:A:18:ASN:N	2.50	0.60
1:A:189:HIS:O	1:A:193:GLN:HG3	2.01	0.60
1:B:167:ASP:OD1	1:B:167:ASP:C	2.43	0.60
1:A:247:PHE:C	1:A:247:PHE:CD2	2.79	0.60
1:B:244:GLU:O	1:B:248:ILE:HG13	2.01	0.60
1:B:240:LEU:CD1	1:B:285:TYR:OH	2.50	0.59
1:A:20:THR:OG1	1:A:21:ASN:N	2.34	0.59
1:A:18:ASN:OD1	1:A:342:PHE:HD2	1.85	0.59
1:A:172:LYS:C	1:A:174:SER:H	2.10	0.58
1:A:354:LYS:HD3	1:A:354:LYS:C	2.28	0.58
1:A:16:GLN:O	1:A:18:ASN:N	2.36	0.58
1:A:49:ASN:C	1:A:49:ASN:ND2	2.59	0.58
1:A:191:VAL:HG12	1:A:219:ARG:NH1	2.17	0.58
1:A:153:ARG:HH22	1:A:232:GLN:NE2	2.02	0.58
1:B:208:THR:HG23	1:B:209:THR:N	2.18	0.57
1:B:198:LEU:HD22	1:B:203:ILE:HD11	1.87	0.57
1:A:191:VAL:HG21	1:A:215:GLU:CG	2.35	0.57
1:A:175:LEU:HB3	1:A:183:VAL:HG21	1.87	0.57
1:B:330:ARG:C	1:B:353:LEU:HD13	2.30	0.56
1:A:227:LYS:HE2	1:A:252:ILE:O	2.06	0.56
1:A:180:THR:CG2	1:A:181:ALA:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:O	1:B:61:ASP:HB2	2.05	0.56
1:A:300:ILE:HG22	1:A:301:THR:CG2	2.36	0.55
1:A:277:THR:O	1:A:280:SER:HB2	2.06	0.55
1:A:335:ARG:O	1:A:336:LEU:HD23	2.07	0.55
1:B:205:PHE:HD1	1:B:232:GLN:HB3	1.70	0.55
1:A:172:LYS:HE3	1:A:172:LYS:HA	1.89	0.55
1:A:19:ASP:O	1:A:20:THR:C	2.49	0.55
1:A:146:VAL:O	1:A:147:GLY:C	2.49	0.55
1:B:220:PRO:O	1:B:224:LEU:HG	2.06	0.55
1:B:178:GLY:C	1:B:180:THR:H	2.15	0.54
1:A:173:ARG:O	1:A:177:GLU:HB2	2.07	0.54
1:A:50:PHE:HB2	1:A:55:ASP:OD2	2.08	0.54
1:B:45:ARG:HD2	1:B:45:ARG:O	2.06	0.54
1:A:284:ILE:HG23	1:A:346:ARG:HD3	1.90	0.54
1:A:68:ILE:O	1:A:68:ILE:CG1	2.54	0.54
1:A:73:ARG:HG2	1:A:104:LYS:HG2	1.89	0.53
1:A:164:ILE:CD1	1:A:166:ILE:HB	2.38	0.53
1:B:94:TYR:CE2	1:B:108:ALA:HB3	2.42	0.53
1:A:342:PHE:O	1:A:343:ALA:HB2	2.08	0.53
1:B:29:ARG:O	1:B:33:SER:HB3	2.08	0.53
1:B:249:ALA:O	1:B:254:PRO:HA	2.08	0.53
1:A:319:SER:OG	1:A:321:TRP:HE3	1.92	0.53
1:A:340:SER:HA	1:A:341:GLY:C	2.24	0.53
1:A:27:LEU:HB3	1:A:318:LEU:CD2	2.38	0.53
1:A:49:ASN:HD22	1:A:50:PHE:HD2	1.56	0.52
1:B:219:ARG:O	1:B:223:VAL:HG23	2.10	0.52
1:B:184:ARG:HD2	1:B:184:ARG:O	2.09	0.52
1:A:41:TRP:CZ2	1:A:68:ILE:HD12	2.45	0.52
1:A:152:GLU:OE2	1:A:156:ARG:NH1	2.40	0.52
1:B:198:LEU:CD2	1:B:203:ILE:HD11	2.40	0.51
1:A:98:GLY:HA2	1:A:102:ALA:HA	1.91	0.51
1:A:172:LYS:C	1:A:174:SER:N	2.66	0.51
1:B:174:SER:O	1:B:175:LEU:C	2.54	0.51
1:A:17:ILE:HG13	1:A:17:ILE:O	2.10	0.51
1:B:97:GLY:C	1:B:99:THR:N	2.69	0.50
1:B:24:VAL:HG21	1:B:59:ILE:HD13	1.94	0.50
1:B:69:SER:O	1:B:71:CYS:N	2.45	0.50
1:A:73:ARG:HG3	1:A:73:ARG:NH1	2.17	0.50
1:A:210:PRO:O	1:A:214:ARG:HB2	2.11	0.50
1:A:336:LEU:HB2	1:A:346:ARG:HB2	1.94	0.50
1:B:28:MET:HE2	1:B:28:MET:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG3	1:A:131:PRO:HD2	1.95	0.49
1:A:5:SER:HA	1:A:8:ILE:HD13	1.93	0.49
1:A:51:ASP:OD1	1:A:54:LYS:HB2	2.12	0.49
1:A:69:SER:O	1:A:70:HIS:C	2.56	0.49
1:A:264:SER:HA	1:A:329:GLU:OE2	2.11	0.49
1:A:301:THR:OG1	1:A:303:GLN:HB2	2.11	0.49
1:B:285:TYR:CE1	1:B:350:ILE:HD12	2.47	0.49
1:B:145:ILE:HG23	1:B:146:VAL:N	2.27	0.49
1:B:30:TRP:CH2	1:B:84:GLY:HA3	2.48	0.49
1:A:4:TYR:C	1:A:8:ILE:CD1	2.86	0.48
1:A:311:GLY:O	1:A:332:THR:HA	2.13	0.48
1:B:94:TYR:HE2	1:B:108:ALA:HB3	1.78	0.48
1:A:300:ILE:HG22	1:A:301:THR:HG23	1.95	0.48
1:B:68:ILE:O	1:B:71:CYS:CB	2.59	0.48
1:A:300:ILE:HD13	1:A:300:ILE:HA	1.65	0.48
1:B:273:SER:HA	1:B:284:ILE:O	2.14	0.48
1:B:121:MET:CE	1:B:156:ARG:HD2	2.42	0.47
1:B:137:ALA:O	1:B:139:ILE:N	2.43	0.47
1:A:130:ARG:NH1	1:A:131:PRO:O	2.47	0.47
1:A:247:PHE:C	1:A:247:PHE:HD2	2.23	0.47
1:B:194:VAL:O	1:B:198:LEU:HG	2.15	0.47
1:A:267:ALA:CB	1:A:317:HIS:HB2	2.43	0.47
1:B:73:ARG:NH1	1:B:102:ALA:CB	2.59	0.47
1:B:127:ARG:NH1	2:B:400:PXC:OAB	2.48	0.47
1:B:130:ARG:HG3	1:B:131:PRO:HD2	1.96	0.47
1:B:190:LEU:O	1:B:191:VAL:C	2.57	0.47
1:B:221:GLU:CD	1:B:221:GLU:N	2.68	0.47
1:B:240:LEU:HD12	1:B:285:TYR:OH	2.14	0.47
1:B:99:THR:HG22	1:B:172:LYS:NZ	2.30	0.47
1:A:28:MET:HG2	1:A:52:PRO:O	2.15	0.47
1:A:180:THR:CG2	1:A:181:ALA:H	2.28	0.47
1:A:74:GLN:NE2	1:B:200:ASN:HD22	2.13	0.46
1:B:233:ILE:HG13	1:B:256:CYS:SG	2.56	0.46
1:A:320:PRO:HD2	1:A:321:TRP:CZ3	2.50	0.46
1:A:120:ARG:HA	1:A:272:ARG:HH11	1.80	0.46
1:B:70:HIS:ND1	1:B:73:ARG:NH2	2.52	0.46
1:B:70:HIS:O	1:B:71:CYS:HB2	2.15	0.46
1:B:109:TYR:CD1	1:B:321:TRP:HB3	2.51	0.46
1:A:124:TYR:O	1:A:125:GLN:C	2.59	0.46
1:A:169:ARG:HD2	1:B:165:ASP:OD2	2.16	0.46
1:A:51:ASP:HA	1:A:52:PRO:HD3	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:HD12	1:A:166:ILE:HB	1.98	0.45
1:B:226:MET:HE2	1:B:253:LEU:CD2	2.46	0.45
1:B:253:LEU:CD1	1:B:256:CYS:HB3	2.47	0.45
1:B:38:SER:HB2	1:B:79:ASN:O	2.17	0.45
1:A:300:ILE:HG22	1:A:301:THR:HG22	1.99	0.45
1:A:313:VAL:O	1:A:314:ILE:HD12	2.17	0.45
1:B:62:LEU:C	1:B:64:GLN:N	2.74	0.45
1:A:27:LEU:HB3	1:A:318:LEU:HD22	1.98	0.45
1:A:153:ARG:HH21	2:A:400:PXC:HAJ	1.81	0.45
1:A:191:VAL:HG12	1:A:219:ARG:CZ	2.47	0.45
1:A:316:THR:HG23	1:A:325:PRO:HA	1.98	0.44
1:A:124:TYR:O	1:A:130:ARG:HD3	2.18	0.44
1:B:232:GLN:HG3	2:B:400:PXC:CAJ	2.47	0.44
1:B:186:TYR:O	1:B:189:HIS:HB3	2.18	0.44
1:A:346:ARG:O	1:A:347:LEU:HD23	2.18	0.44
1:B:216:LEU:HD13	1:B:222:VAL:HG11	1.99	0.44
1:A:49:ASN:ND2	1:A:50:PHE:HD2	2.16	0.44
1:A:54:LYS:O	1:A:57:LYS:HE3	2.17	0.44
1:A:77:VAL:O	1:A:78:ALA:C	2.60	0.44
1:B:320:PRO:HD2	1:B:321:TRP:CZ3	2.53	0.44
1:A:172:LYS:O	1:A:174:SER:N	2.51	0.44
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.72	0.44
1:A:54:LYS:HD3	1:A:54:LYS:HA	1.81	0.44
1:A:74:GLN:HE21	1:A:74:GLN:CA	2.15	0.43
1:A:89:SER:O	1:A:90:HIS:HB2	2.18	0.43
1:A:74:GLN:NE2	1:B:200:ASN:ND2	2.65	0.43
1:B:125:GLN:HG3	1:B:126:HIS:CE1	2.53	0.43
1:B:327:VAL:H	1:B:327:VAL:HG23	1.51	0.43
1:B:187:THR:HG22	1:B:215:GLU:OE1	2.18	0.43
1:B:247:PHE:CE1	1:B:251:GLU:HG2	2.52	0.43
1:B:157:LEU:HA	1:B:157:LEU:HD23	1.76	0.43
1:B:203:ILE:HD13	1:B:203:ILE:H	1.83	0.43
1:A:115:ALA:O	1:A:116:LEU:C	2.60	0.43
1:B:212:VAL:O	1:B:216:LEU:HB2	2.18	0.43
1:A:28:MET:CE	1:A:56:VAL:HG11	2.39	0.43
1:B:76:PRO:O	1:B:77:VAL:C	2.61	0.43
1:B:83:GLN:H	1:B:83:GLN:HG3	1.50	0.43
1:B:120:ARG:O	1:B:120:ARG:HG3	2.18	0.43
1:B:270:VAL:HG23	1:B:270:VAL:O	2.19	0.43
1:A:249:ALA:O	1:A:254:PRO:HA	2.18	0.43
1:B:315:VAL:O	1:B:315:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASN:O	1:B:63:ARG:HG3	2.18	0.42
1:A:130:ARG:HA	1:A:131:PRO:HD3	1.81	0.42
1:A:191:VAL:HG21	1:A:215:GLU:HB3	2.01	0.42
1:A:73:ARG:HH11	1:A:73:ARG:CG	2.22	0.42
1:A:195:GLN:O	1:A:199:MET:HG2	2.19	0.42
1:B:59:ILE:HD13	1:B:59:ILE:HA	1.73	0.42
1:A:82:PRO:HD2	1:A:85:LEU:HD11	2.01	0.42
1:A:290:PRO:O	1:A:291:PHE:C	2.62	0.42
1:B:208:THR:OG1	1:B:209:THR:N	2.52	0.42
1:A:303:GLN:O	1:A:304:THR:C	2.61	0.42
1:A:27:LEU:CB	1:A:318:LEU:HD22	2.50	0.42
1:A:67:ASP:HB2	1:A:326:ARG:O	2.19	0.42
1:B:268:LEU:HD12	1:B:317:HIS:CE1	2.55	0.42
1:A:171:VAL:O	1:A:175:LEU:HD13	2.20	0.42
1:A:290:PRO:CD	1:A:291:PHE:H	2.29	0.42
1:B:145:ILE:CG2	1:B:146:VAL:N	2.82	0.41
1:A:55:ASP:OD1	1:A:55:ASP:N	2.53	0.41
1:B:253:LEU:HD11	1:B:258:PHE:CZ	2.54	0.41
1:A:290:PRO:CD	1:A:291:PHE:N	2.78	0.41
1:A:7:GLU:O	1:A:10:ALA:HB3	2.19	0.41
1:A:317:HIS:CD2	1:A:317:HIS:C	2.99	0.41
1:B:51:ASP:O	1:B:52:PRO:C	2.63	0.41
1:B:62:LEU:C	1:B:64:GLN:H	2.29	0.41
1:B:218:LYS:O	1:B:220:PRO:HD2	2.20	0.41
1:B:310:ARG:HA	1:B:334:ILE:HA	2.01	0.41
1:A:320:PRO:HD2	1:A:321:TRP:CE3	2.56	0.41
1:A:29:ARG:O	1:A:33:SER:HB2	2.20	0.41
1:A:58:THR:O	1:A:61:ASP:HB2	2.20	0.41
1:A:121:MET:HA	1:A:124:TYR:CZ	2.56	0.41
1:B:69:SER:O	1:B:70:HIS:C	2.63	0.41
1:A:100:THR:HG22	1:A:101:GLY:H	1.85	0.41
1:B:173:ARG:O	1:B:174:SER:C	2.63	0.41
1:A:49:ASN:ND2	1:A:49:ASN:O	2.54	0.41
1:B:38:SER:O	1:B:39:PRO:C	2.64	0.40
1:B:219:ARG:HA	1:B:220:PRO:HD2	1.85	0.40
1:B:331:ASP:N	1:B:353:LEU:HD13	2.36	0.40
1:A:144:HIS:HE2	1:B:165:ASP:CG	2.28	0.40
1:A:191:VAL:HG21	1:A:215:GLU:CB	2.51	0.40
1:B:121:MET:HE1	1:B:156:ARG:CB	2.52	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	350/366 (96%)	297 (85%)	43 (12%)	10 (3%)	3	13
1	B	350/366 (96%)	299 (85%)	37 (11%)	14 (4%)	2	8
All	All	700/732 (96%)	596 (85%)	80 (11%)	24 (3%)	3	11

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	20	THR
1	A	34	LYS
1	A	56	VAL
1	A	340	SER
1	B	98	GLY
1	B	102	ALA
1	B	125	GLN
1	B	138	ALA
1	B	179	ASP
1	A	97	GLY
1	B	71	CYS
1	B	100	THR
1	B	166	ILE
1	B	180	THR
1	A	18	ASN
1	A	103	PRO
1	B	69	SER
1	B	328	ALA
1	B	77	VAL
1	B	195	GLN
1	B	220	PRO
1	A	35	GLU
1	A	341	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	304/316 (96%)	245 (81%)	59 (19%)	1	5
1	B	304/316 (96%)	256 (84%)	48 (16%)	2	9
All	All	608/632 (96%)	501 (82%)	107 (18%)	2	7

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	13	LYS
1	A	16	GLN
1	A	17	ILE
1	A	18	ASN
1	A	20	THR
1	A	21	ASN
1	A	34	LYS
1	A	38	SER
1	A	42	LEU
1	A	49	ASN
1	A	51	ASP
1	A	54	LYS
1	A	55	ASP
1	A	56	VAL
1	A	57	LYS
1	A	59	ILE
1	A	62	LEU
1	A	68	ILE
1	A	70	HIS
1	A	73	ARG
1	A	74	GLN
1	A	83	GLN
1	A	92	GLN
1	A	99	THR
1	A	100	THR
1	A	118	SER

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Mol	Chain	Res	Type
1	A	130	ARG
1	A	141	THR
1	A	145	ILE
1	A	151	LYS
1	A	156	ARG
1	A	164	ILE
1	A	170	TRP
1	A	172	LYS
1	A	175	LEU
1	A	187	THR
1	A	189	HIS
1	A	215	GLU
1	A	220	PRO
1	A	228	GLN
1	A	234	THR
1	A	240	LEU
1	A	241	ASN
1	A	272	ARG
1	A	275	LEU
1	A	280	SER
1	A	281	GLN
1	A	284	ILE
1	A	300	ILE
1	A	305	VAL
1	A	306	GLU
1	A	309	GLU
1	A	314	ILE
1	A	318	LEU
1	A	319	SER
1	A	339	VAL
1	A	350	ILE
1	A	354	LYS
1	B	5	SER
1	B	20	THR
1	B	33	SER
1	B	34	LYS
1	B	42	LEU
1	B	53	ILE
1	B	57	LYS
1	B	60	ASN
1	B	66	SER
1	B	73	ARG

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Mol	Chain	Res	Type
1	B	77	VAL
1	B	122	SER
1	B	130	ARG
1	B	139	ILE
1	B	141	THR
1	B	151	LYS
1	B	160	MET
1	B	166	ILE
1	B	175	LEU
1	B	184	ARG
1	B	185	LYS
1	B	195	GLN
1	B	202	ASP
1	B	203	ILE
1	B	212	VAL
1	B	216	LEU
1	B	221	GLU
1	B	227	LYS
1	B	228	GLN
1	B	246	LYS
1	B	251	GLU
1	B	252	ILE
1	B	265	THR
1	B	273	SER
1	B	275	LEU
1	B	277	THR
1	B	279	GLU
1	B	292	ILE
1	B	297	VAL
1	B	299	SER
1	B	310	ARG
1	B	317	HIS
1	B	318	LEU
1	B	327	VAL
1	B	330	ARG
1	B	340	SER
1	B	351	GLU
1	B	353	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	21	ASN
1	A	49	ASN
1	A	74	GLN
1	A	83	GLN
1	A	92	GLN
1	A	193	GLN
1	A	195	GLN
1	A	228	GLN
1	A	232	GLN
1	A	281	GLN
1	A	282	GLN
1	B	16	GLN
1	B	18	ASN
1	B	25	GLN
1	B	74	GLN
1	B	79	ASN
1	B	150	ASN
1	B	193	GLN
1	B	200	ASN
1	B	228	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](#)

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	PXC	B	400	-	22,22,22	1.40	3 (13%)	32,32,32	1.67	4 (12%)
2	PXC	A	400	-	22,22,22	1.40	3 (13%)	32,32,32	1.79	5 (15%)

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	PXC	B	400	-	-	4/8/8/8	0/3/3/3
2	PXC	A	400	-	-	4/8/8/8	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PXC	CAO-CAM	2.94	1.55	1.50
2	A	400	PXC	CAP-CAN	2.51	1.54	1.50
2	A	400	PXC	CAO-CAM	2.49	1.54	1.50
2	B	400	PXC	CAP-CAN	2.46	1.54	1.50
2	A	400	PXC	CAF-CAJ	2.33	1.41	1.36
2	B	400	PXC	CAE-CAI	2.02	1.41	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PXC	CAS-NAK-CAR	4.49	122.57	116.96
2	A	400	PXC	CAT-NAL-CAQ	4.38	122.43	116.96
2	B	400	PXC	CAT-NAL-CAQ	4.18	122.18	116.96
2	B	400	PXC	CAS-NAK-CAR	4.07	122.05	116.96
2	A	400	PXC	CAQ-CAS-NAK	-3.75	117.98	121.54
2	A	400	PXC	CAR-CAT-NAL	-3.72	118.01	121.54
2	B	400	PXC	CAQ-CAS-NAK	-3.66	118.07	121.54
2	B	400	PXC	CAR-CAT-NAL	-3.54	118.18	121.54
2	A	400	PXC	OAD-CAN-CAP	2.05	119.79	114.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

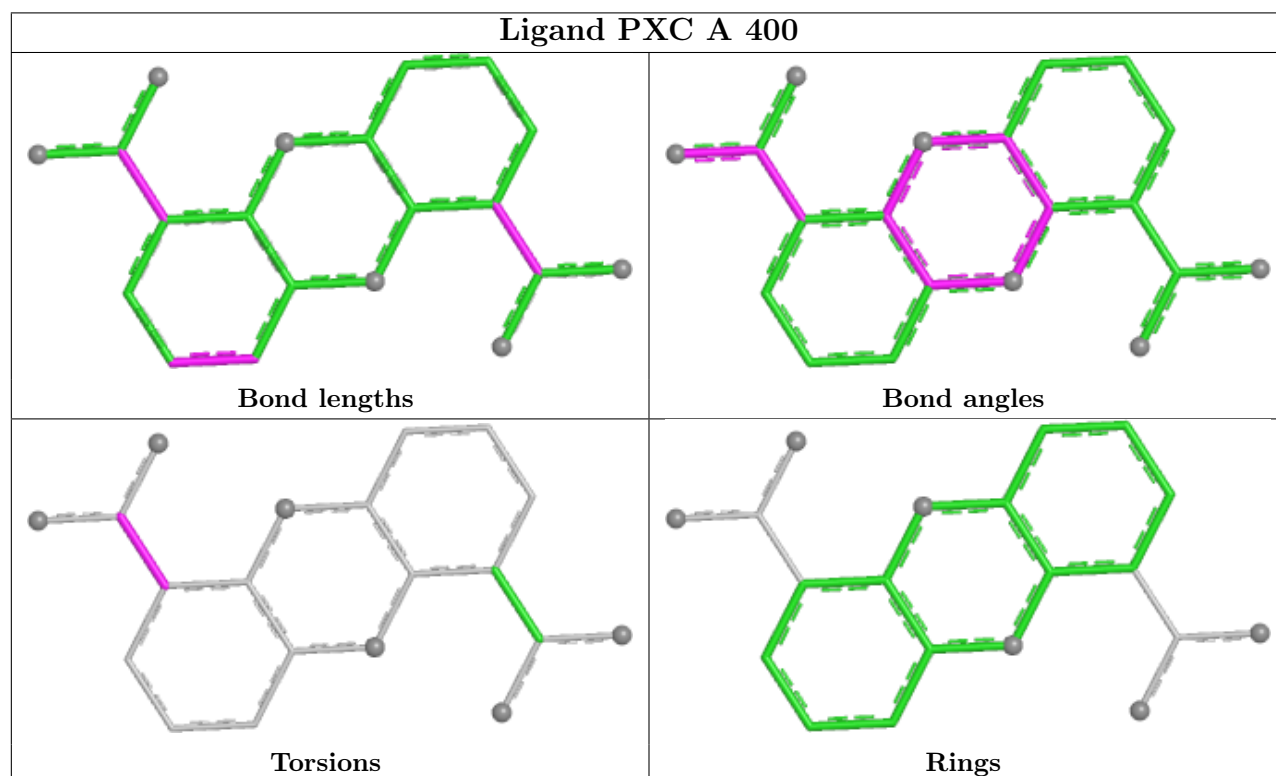
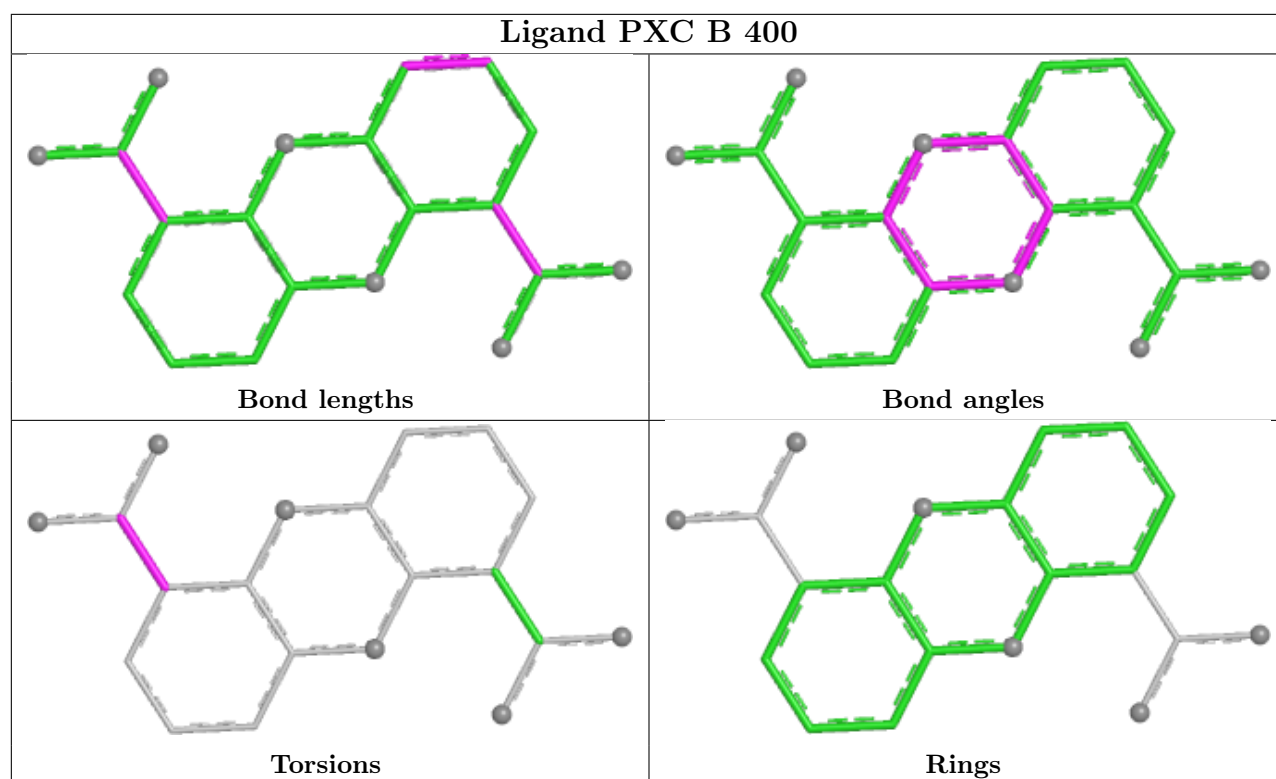
Mol	Chain	Res	Type	Atoms
2	A	400	PXC	OAB-CAN-CAP-CAT
2	A	400	PXC	OAD-CAN-CAP-CAT
2	B	400	PXC	OAB-CAN-CAP-CAT
2	B	400	PXC	OAD-CAN-CAP-CAT
2	A	400	PXC	OAB-CAN-CAP-CAH
2	A	400	PXC	OAD-CAN-CAP-CAH
2	B	400	PXC	OAB-CAN-CAP-CAH
2	B	400	PXC	OAD-CAN-CAP-CAH

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	PXC	3	0
2	A	400	PXC	2	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 than 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.



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

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	352/366 (96%)	-0.14	11 (3%)	51	41	14, 34, 59, 68	0
1	B	352/366 (96%)	-0.11	20 (5%)	29	22	15, 35, 56, 69	3 (0%)
All	All	704/732 (96%)	-0.12	31 (4%)	39	31	14, 34, 57, 69	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	SER	11.2
1	B	103	PRO	7.3
1	B	101	GLY	5.1
1	B	3	ASP	4.9
1	B	102	ALA	4.7
1	B	97	GLY	4.5
1	B	99	THR	4.0
1	B	128	PRO	3.4
1	B	100	THR	3.2
1	B	215	GLU	3.2
1	B	173	ARG	2.9
1	B	98	GLY	2.9
1	A	29	ARG	2.8
1	B	155	LEU	2.7
1	A	4	TYR	2.7
1	B	169	ARG	2.5
1	A	239	GLU	2.5
1	A	36	THR	2.4
1	B	129	GLY	2.4
1	B	219	ARG	2.4
1	B	70	HIS	2.4
1	B	354	LYS	2.3
1	A	97	GLY	2.3
1	A	7	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	THR	2.3
1	A	339	VAL	2.2
1	B	216	LEU	2.2
1	B	124	TYR	2.1
1	A	173	ARG	2.1
1	A	20	THR	2.0
1	A	343	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

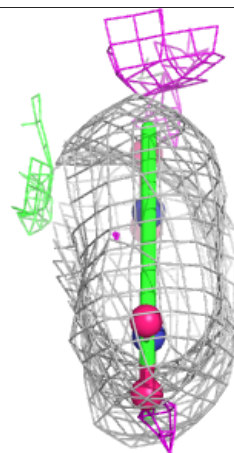
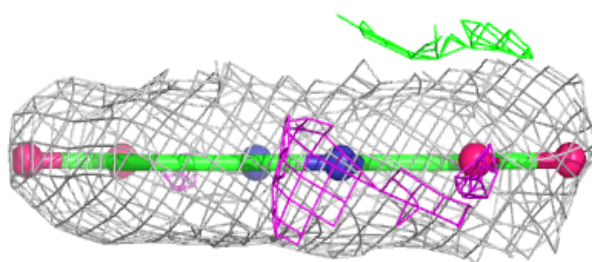
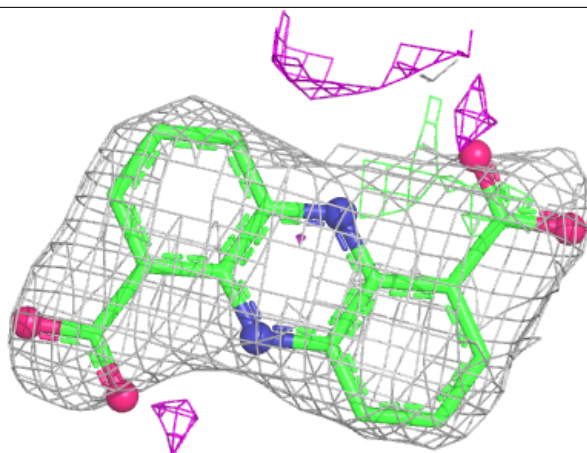
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PXC	B	400	20/20	0.86	0.12	67,68,71,73	0
2	PXC	A	400	20/20	0.91	0.09	44,46,51,55	0

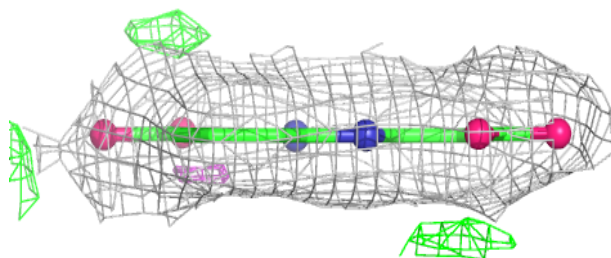
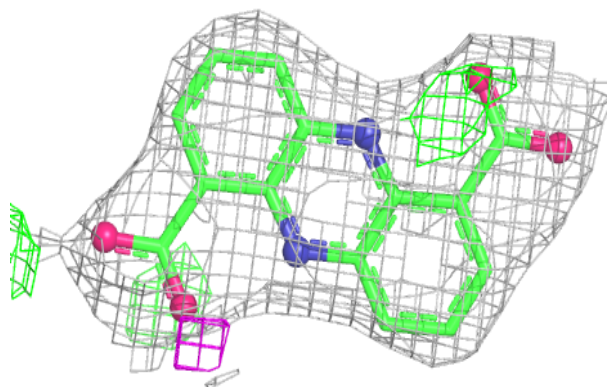
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PXC B 400:

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

**Electron density around PXC A 400:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.