



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 02:38 PM BST

PDB ID : 3L2K
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 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 : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

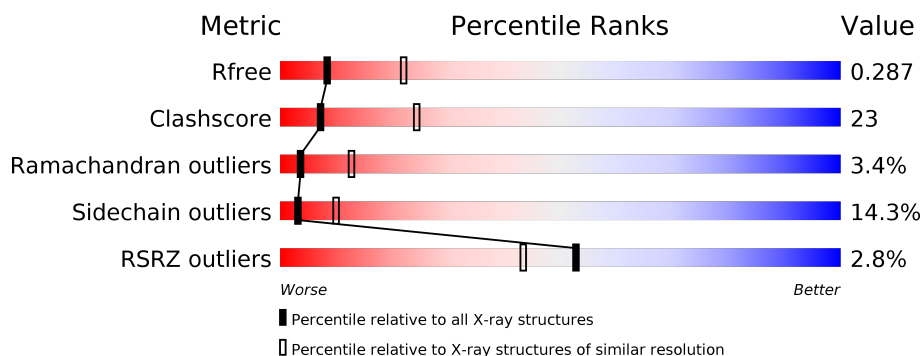
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>30%</div> <div>9%</div> <div>• •</div> </div> </div>
1	B	366	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>8%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

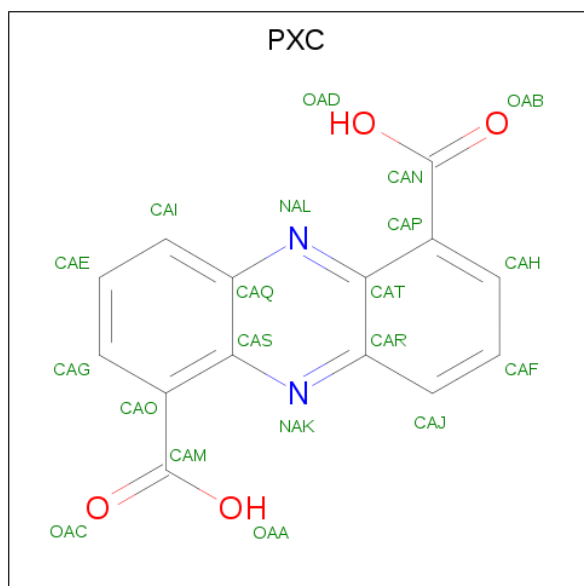
There are 3 unique types of molecules in this entry. The entry contains 5594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: 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		

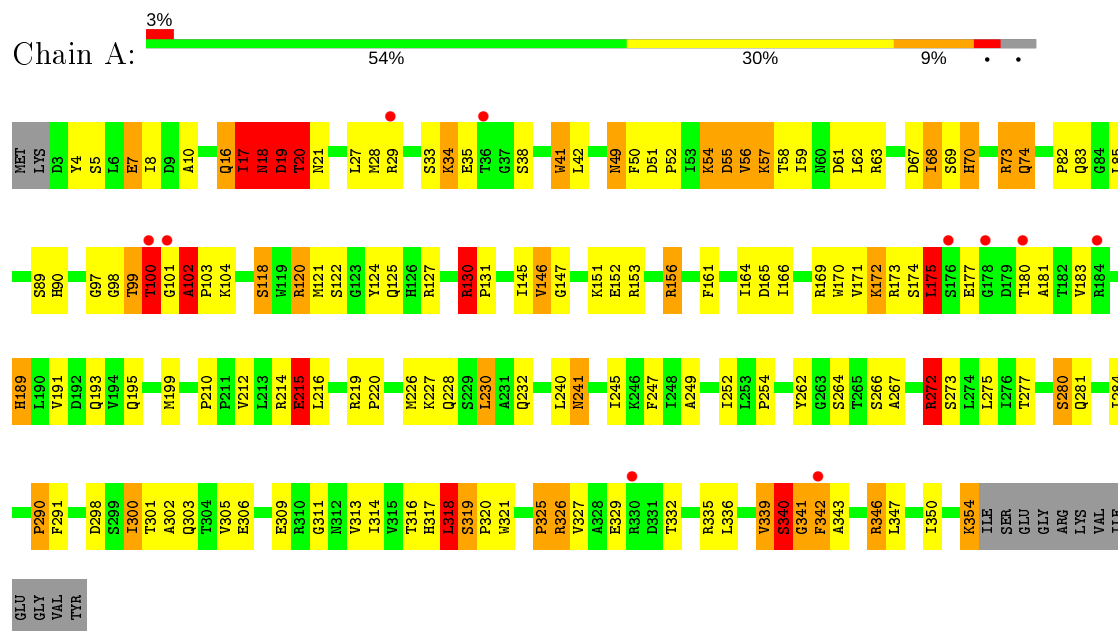
- Molecule 3 is water.

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

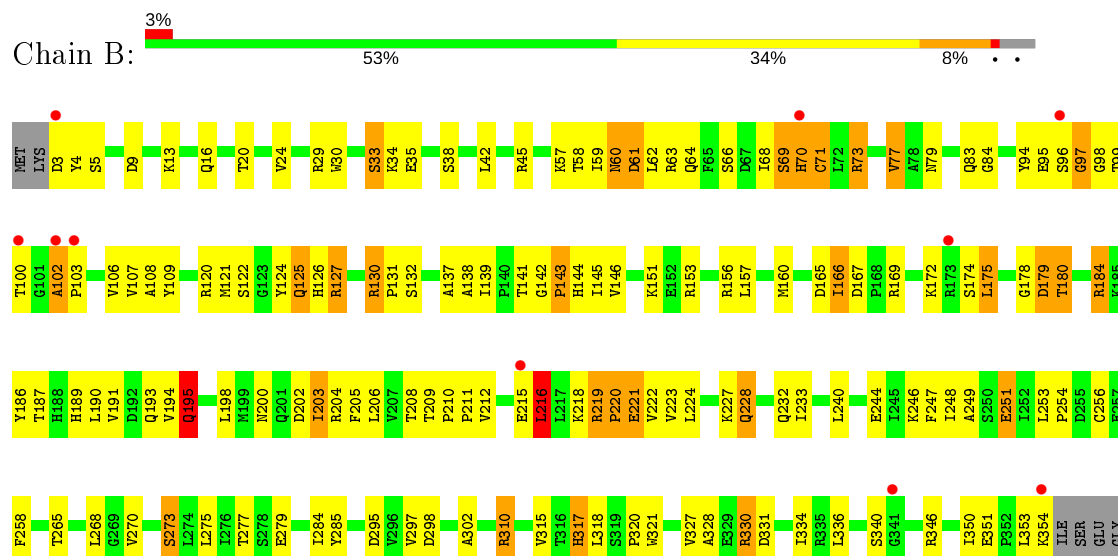
3 Residue-property plots

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: Ehpf



• Molecule 1: Ehpf



ARG
LYS
VAL
ILE
GLU
GLY
VAL
TYR

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 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (26.78-2.80) 99.9 (26.78-2.80)	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 (5.09%)	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)	0.33 , 45.0	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	0.94	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 [i](#)

5.1 Standard geometry [i](#)

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	1.34	9/2834 (0.3%)	1.32	23/3857 (0.6%)
1	B	1.31	10/2834 (0.4%)	1.26	11/3857 (0.3%)
All	All	1.33	19/5668 (0.3%)	1.29	34/7714 (0.4%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	3	ASP	N-CA	6.99	1.60	1.46
1	B	354	LYS	C-O	6.08	1.34	1.23
1	A	122	SER	C-O	6.05	1.34	1.23
1	B	219	ARG	CZ-NH1	5.83	1.40	1.33
1	A	161	PHE	CD2-CE2	5.67	1.50	1.39
1	B	107	VAL	CB-CG2	-5.63	1.41	1.52
1	A	262	TYR	CD2-CE2	-5.55	1.31	1.39
1	B	35	GLU	CB-CG	-5.52	1.41	1.52
1	A	146	VAL	CB-CG2	5.48	1.64	1.52
1	B	106	VAL	CB-CG1	-5.47	1.41	1.52
1	A	215	GLU	CD-OE1	5.44	1.31	1.25
1	B	9	ASP	CB-CG	5.44	1.63	1.51
1	B	35	GLU	CD-OE1	5.43	1.31	1.25
1	B	4	TYR	CD2-CE2	5.36	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	TRP	CE3-CZ3	5.33	1.47	1.38
1	A	212	VAL	CB-CG1	-5.21	1.42	1.52
1	A	245	ILE	CA-CB	-5.17	1.43	1.54
1	A	342	PHE	CB-CG	5.10	1.60	1.51
1	B	143	PRO	N-CD	5.06	1.54	1.47

All (34) 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	A	120	ARG	NE-CZ-NH1	-8.25	116.18	120.30
1	B	143	PRO	CA-N-CD	-8.01	100.29	111.50
1	A	318	LEU	CB-CG-CD2	8.00	124.60	111.00
1	A	175	LEU	CA-CB-CG	7.80	133.25	115.30
1	A	156	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	B	142	GLY	C-N-CD	7.16	143.44	128.40
1	A	102	ALA	C-N-CD	-7.04	105.12	120.60
1	A	120	ARG	NE-CZ-NH2	7.00	123.80	120.30
1	A	215	GLU	OE1-CD-OE2	6.03	130.54	123.30
1	A	102	ALA	C-N-CA	5.96	147.03	122.00
1	A	118	SER	N-CA-CB	5.91	119.36	110.50
1	B	204	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	96	SER	N-CA-C	-5.80	95.33	111.00
1	A	272	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	326	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	340	SER	N-CA-C	5.58	126.06	111.00
1	A	130	ARG	CG-CD-NE	5.50	123.35	111.80
1	B	206	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	A	281	GLN	CB-CA-C	5.37	121.13	110.40
1	B	61	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	19	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	3	ASP	N-CA-C	5.32	125.37	111.00
1	A	165	ASP	CB-CG-OD1	-5.31	113.52	118.30
1	A	156	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	272	ARG	CG-CD-NE	-5.26	100.74	111.80
1	A	230	LEU	CA-CB-CG	-5.24	103.26	115.30
1	B	298	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	35	GLU	OE1-CD-OE2	5.19	129.53	123.30
1	B	3	ASP	CB-CG-OD2	5.18	122.97	118.30
1	A	346	ARG	CB-CA-C	-5.15	100.10	110.40
1	B	216	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	127	ARG	NE-CZ-NH1	-5.06	117.77	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	SER	C-N-CA	-5.04	111.71	122.30

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	141	0
1	B	2769	0	2737	119	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	250	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 23.

All (250) 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:HH11	1:B:184:ARG:HG3	1.13	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:16:GLN:HE21	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:HE21	1:B:228:GLN:HA	1.22	1.02
1:A:193:GLN:HE21	1:B:169:ARG:HH11	1.07	0.97
1:B:228:GLN:NE2	1:B:228:GLN:HA	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
1:B:102:ALA:CB	1:B:103:PRO:HA	2.02	0.88
1:B:130:ARG:CG	1:B:130:ARG:HH11	1.89	0.85
1:A:73:ARG:HH11	1:A:73:ARG:HG3	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:241:ASN:C	1:A:241:ASN:OD1	2.16	0.83
1:A:16:GLN:HE21	1:A:16:GLN:H	1.23	0.82
1:A:16:GLN:C	1:A:18:ASN:H	1.83	0.81
1:B:153:ARG:HH21	2:B:400:PXC:HAJ	1.45	0.81
1:B:253:LEU:HD12	1:B:253:LEU:O	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:NE2	1:A:16:GLN:H	1.83	0.77
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	1:B:184:ARG:HH11	1.95	0.72
1:A:63:ARG:NH2	1:A:302:ALA:O	2.23	0.72
1:A:56:VAL:HG12	1:A:56:VAL:O	1.87	0.71
1:B:228:GLN:HE21	1:B:228:GLN:C	1.92	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:NH1	1:B:184:ARG:HG3	1.94	0.69
1:A:298:ASP:OD2	1:A:301:THR:HG23	1.93	0.68
1:A:49:ASN:HD22	1:A:49:ASN:C	1.98	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:290:PRO:HD2	1:A:291:PHE:N	2.11	0.66
1:A:266:SER:OG	1:A:327:VAL:HG21	1.96	0.65
1:A:267:ALA:HB1	1:A:317:HIS:HB2	1.78	0.65
1:A:16:GLN:C	1:A:18:ASN:N	2.50	0.64
1:B:121:MET:HE1	1:B:156:ARG:HD2	1.78	0.64
1:A:180:THR:HG23	1:A:181:ALA:N	2.11	0.64
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: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:B:221:GLU:H	1:B:221:GLU:CD	2.01	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:210:PRO:HD2	1:B:211:PRO:HD3	1.81	0.61
1:A:16:GLN:N	1:A:16:GLN:NE2	2.35	0.61
1:A:191:VAL:HG21	1:A:215:GLU:HG3	1.83	0.61
1:A:74:GLN:HA	1:A:74:GLN:NE2	2.11	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:A:189:HIS:O	1:A:193:GLN:HG3	2.01	0.60
1:A:20:THR:OG1	1:A:21:ASN:N	2.34	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:OD1	1:A:342:PHE:HD2	1.85	0.59
1:A:16:GLN:O	1:A:18:ASN:N	2.36	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:A:4:TYR:C	1:A:8:ILE:HD12	2.21	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: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
1:B:317:HIS:C	1:B:317:HIS:CD2	2.80	0.56
1:B:167:ASP:OD1	1:B:167:ASP:C	2.43	0.56
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:247:PHE:C	1:A:247:PHE:CD2	2.79	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:A:49:ASN:ND2	1:A:49:ASN:C	2.59	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:B:220:PRO:O	1:B:224:LEU:HG	2.06	0.55
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:O	1:B:45:ARG:HD2	2.06	0.54
1:A:284:ILE:HG23	1:A:346:ARG:HD3	1.90	0.54
1:A:172:LYS:C	1:A:174:SER:H	2.10	0.54
1:A:68:ILE:CG1	1:A:68:ILE:O	2.54	0.54
1:A:354:LYS:C	1:A:354:LYS:HD3	2.28	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: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:O	1:B:184:ARG:HD2	2.09	0.52
1:A:28:MET:CE	1:A:56:VAL:HG11	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:OE2	1:A:156:ARG:NH1	2.40	0.52
1:A:41:TRP:CZ2	1:A:68:ILE:HD12	2.45	0.52
1:B:330:ARG:C	1:B:353:LEU:HD13	2.30	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:17:ILE:HG13	1:A:17:ILE:O	2.10	0.51
1:B:24:VAL:HG21	1:B:59:ILE:HD13	1.94	0.50
1:A:146:VAL:O	1:A:147:GLY:C	2.49	0.50
1:A:19:ASP:O	1:A:20:THR:C	2.49	0.50
1:B:69:SER:O	1:B:71:CYS:N	2.45	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:A:73:ARG:NH1	1:A:73:ARG:HG3	2.17	0.50
1:B:178:GLY:C	1:B:180:THR:H	2.15	0.50
1:A:130:ARG:HG3	1:A:131:PRO:HD2	1.95	0.49
1:A:264:SER:HA	1:A:329:GLU:OE2	2.11	0.49
1:A:51:ASP:OD1	1:A:54:LYS:HB2	2.12	0.49
1:A:5:SER:HA	1:A:8:ILE:HD13	1.93	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:28:MET:HE2	1:A:56:VAL:HG11	1.95	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:137:ALA:O	1:B:139:ILE:N	2.43	0.47
1:B:121:MET:CE	1:B:156:ARG:HD2	2.42	0.47
1:A:130:ARG:NH1	1:A:131:PRO:O	2.47	0.47
1:A:172:LYS:C	1:A:174:SER:N	2.66	0.47
1:B:194:VAL:O	1:B:198:LEU:HG	2.15	0.47
1:B:221:GLU:N	1:B:221:GLU:CD	2.68	0.47
1:A:267:ALA:CB	1:A:317:HIS:HB2	2.43	0.47
1:B:127:ARG:NH1	2:B:400:PXC:OAB	2.48	0.47
1:B:73:ARG:NH1	1:B:102:ALA:CB	2.59	0.47
1:B:130:ARG:HG3	1:B:131:PRO:HD2	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:THR:CG2	1:A:181:ALA:H	2.28	0.47
1:A:28:MET:HG2	1:A:52:PRO:O	2.15	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:109:TYR:CD1	1:B:321:TRP:HB3	2.51	0.46
1:B:174:SER:O	1:B:175:LEU:C	2.54	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:97:GLY:C	1:B:99:THR:N	2.69	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
1:A:164:ILE:HD12	1:A:166:ILE:HB	1.98	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:A:191:VAL:HG12	1:A:219:ARG:CZ	2.47	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:69:SER:O	1:A:70:HIS:C	2.56	0.45
1:A:28:MET:HE1	1:A:62:LEU:CD2	2.47	0.44
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:4:TYR:C	1:A:8:ILE:CD1	2.86	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:CA	1:A:74:GLN:HE21	2.15	0.43
1:A:89:SER:O	1:A:90:HIS:HB2	2.18	0.43
1:B:125:GLN:HG3	1:B:126:HIS:CE1	2.53	0.43
1:A:74:GLN:NE2	1:B:200:ASN:ND2	2.65	0.43
1:B:327:VAL:HG23	1:B:327:VAL:H	1.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:203:ILE:HD13	1.83	0.43
1:B:212:VAL:O	1:B:216:LEU:HB2	2.18	0.43
1:B:120:ARG:HG3	1:B:120:ARG:O	2.18	0.43
1:B:270:VAL:O	1:B:270:VAL:HG23	2.19	0.43
1:B:83:GLN:HG3	1:B:83:GLN:H	1.50	0.43
1:A:249:ALA:O	1:A:254:PRO:HA	2.18	0.43
1:B:315:VAL:HG13	1:B:315:VAL:O	2.19	0.43
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:195:GLN:O	1:A:199:MET:HG2	2.19	0.42
1:A:73:ARG:HH11	1:A:73:ARG:CG	2.22	0.42
1:B:59:ILE:HA	1:B:59:ILE:HD13	1.73	0.42
1:A:82:PRO:HD2	1:A:85:LEU:HD11	2.01	0.42
1:B:190:LEU:O	1:B:191:VAL:C	2.57	0.42
1:B:208:THR:OG1	1:B:209:THR:N	2.52	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:N	1:A:55:ASP:OD1	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: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:124:TYR:O	1:A:125:GLN:C	2.59	0.41
1:A:247:PHE:C	1:A:247:PHE:HD2	2.23	0.41
1:A:320:PRO:HD2	1:A:321:TRP:CE3	2.56	0.41
1:A:121:MET:HA	1:A:124:TYR:CZ	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:B:121:MET:HE1	1:B:156:ARG:CB	2.51	0.41
1:A:100:THR:HG22	1:A:101:GLY:H	1.85	0.41
1:B:62:LEU:C	1:B:64:GLN:N	2.74	0.41
1:A:49:ASN:O	1:A:49:ASN:ND2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:VAL:HG21	1:A:215:GLU:CB	2.51	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	350/366 (96%)	297 (85%)	43 (12%)	10 (3%)	4	15
1	B	350/366 (96%)	299 (85%)	37 (11%)	14 (4%)	3	9
All	All	700/732 (96%)	596 (85%)	80 (11%)	24 (3%)	3	13

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	259 (85%)	45 (15%)	3	9
1	B	304/316 (96%)	262 (86%)	42 (14%)	3	11
All	All	608/632 (96%)	521 (86%)	87 (14%)	3	10

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	16	GLN
1	A	17	ILE
1	A	18	ASN
1	A	20	THR
1	A	34	LYS
1	A	38	SER
1	A	42	LEU
1	A	49	ASN
1	A	54	LYS
1	A	55	ASP
1	A	57	LYS
1	A	59	ILE
1	A	68	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	70	HIS
1	A	73	ARG
1	A	74	GLN
1	A	83	GLN
1	A	99	THR
1	A	100	THR
1	A	118	SER
1	A	130	ARG
1	A	145	ILE
1	A	151	LYS
1	A	170	TRP
1	A	172	LYS
1	A	175	LEU
1	A	189	HIS
1	A	215	GLU
1	A	220	PRO
1	A	228	GLN
1	A	240	LEU
1	A	241	ASN
1	A	272	ARG
1	A	275	LEU
1	A	280	SER
1	A	300	ILE
1	A	305	VAL
1	A	306	GLU
1	A	309	GLU
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	13	LYS
1	B	16	GLN
1	B	20	THR
1	B	33	SER
1	B	34	LYS
1	B	42	LEU
1	B	57	LYS
1	B	60	ASN
1	B	66	SER
1	B	73	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	VAL
1	B	122	SER
1	B	127	ARG
1	B	130	ARG
1	B	141	THR
1	B	151	LYS
1	B	160	MET
1	B	166	ILE
1	B	175	LEU
1	B	179	ASP
1	B	184	ARG
1	B	195	GLN
1	B	202	ASP
1	B	203	ILE
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	265	THR
1	B	273	SER
1	B	275	LEU
1	B	277	THR
1	B	279	GLU
1	B	310	ARG
1	B	317	HIS
1	B	318	LEU
1	B	330	ARG
1	B	340	SER
1	B	351	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	49	ASN
1	A	74	GLN
1	A	79	ASN
1	A	83	GLN
1	A	92	GLN
1	A	193	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	232	GLN
1	A	281	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	195	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 monosaccharides 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	-	18,22,22	2.80	2 (11%)	22,32,32	2.12	8 (36%)
2	PXC	A	400	-	18,22,22	2.72	5 (27%)	22,32,32	2.25	8 (36%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PXC	CAO-CAM	8.23	1.55	1.47
2	A	400	PXC	CAP-CAN	7.49	1.54	1.47
2	A	400	PXC	CAO-CAM	7.47	1.54	1.47
2	B	400	PXC	CAP-CAN	7.41	1.54	1.47
2	A	400	PXC	CAF-CAJ	2.17	1.41	1.36
2	A	400	PXC	CAG-CAO	2.03	1.42	1.38
2	A	400	PXC	CAH-CAP	2.00	1.41	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PXC	CAS-NAK-CAR	4.88	122.57	117.02
2	A	400	PXC	CAT-NAL-CAQ	4.75	122.43	117.02
2	B	400	PXC	CAT-NAL-CAQ	4.53	122.18	117.02
2	B	400	PXC	CAS-NAK-CAR	4.42	122.05	117.02
2	A	400	PXC	CAQ-CAS-NAK	-4.03	117.98	121.56
2	A	400	PXC	CAR-CAT-NAL	-4.00	118.01	121.56
2	B	400	PXC	CAQ-CAS-NAK	-3.93	118.07	121.56
2	B	400	PXC	CAR-CAT-NAL	-3.80	118.18	121.56
2	A	400	PXC	CAO-CAS-NAK	2.81	122.11	118.94
2	B	400	PXC	CAO-CAS-NAK	2.56	121.83	118.94
2	A	400	PXC	CAS-CAQ-NAL	-2.54	119.45	121.35
2	A	400	PXC	CAP-CAT-NAL	2.47	121.73	118.94
2	B	400	PXC	CAP-CAT-NAL	2.42	121.67	118.94
2	A	400	PXC	CAT-CAR-NAK	-2.39	119.56	121.35
2	B	400	PXC	CAS-CAQ-NAL	-2.17	119.72	121.35
2	B	400	PXC	CAT-CAR-NAK	-2.08	119.79	121.35

There are no chirality outliers.

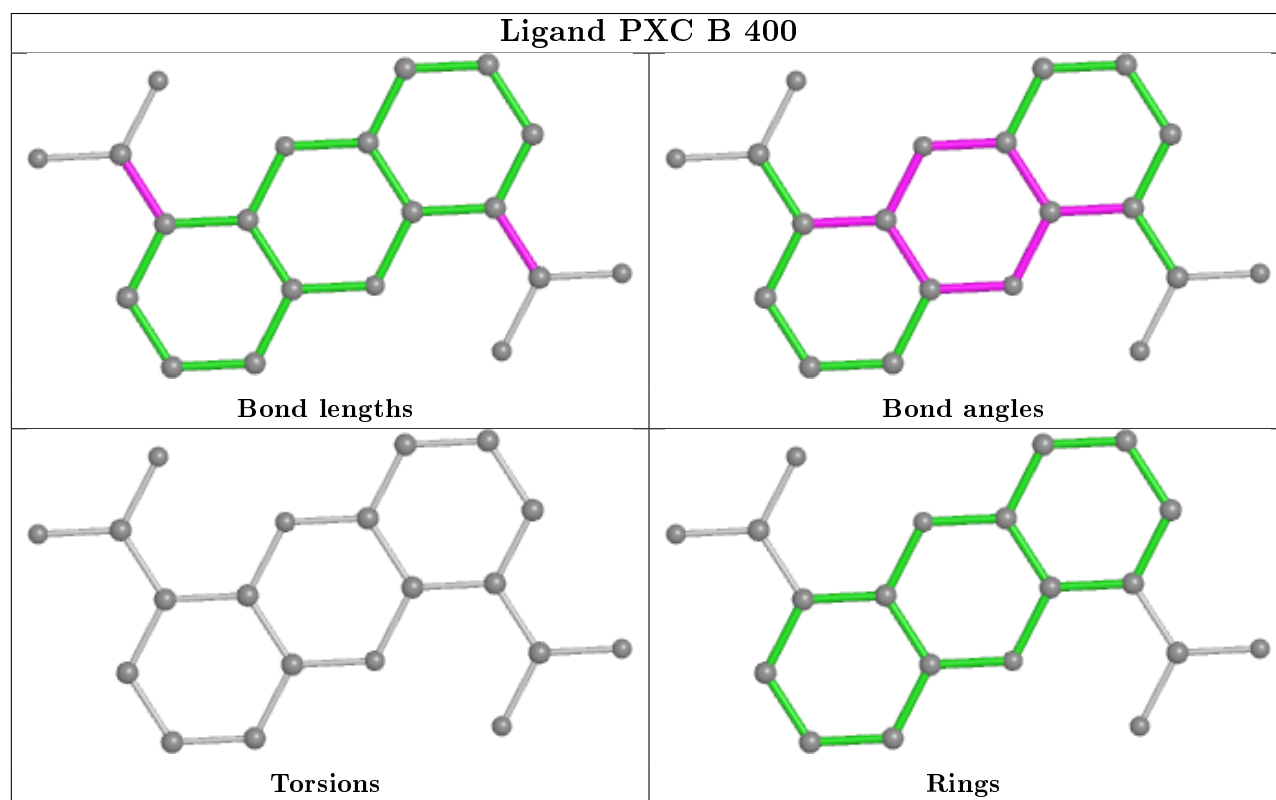
There are no torsion outliers.

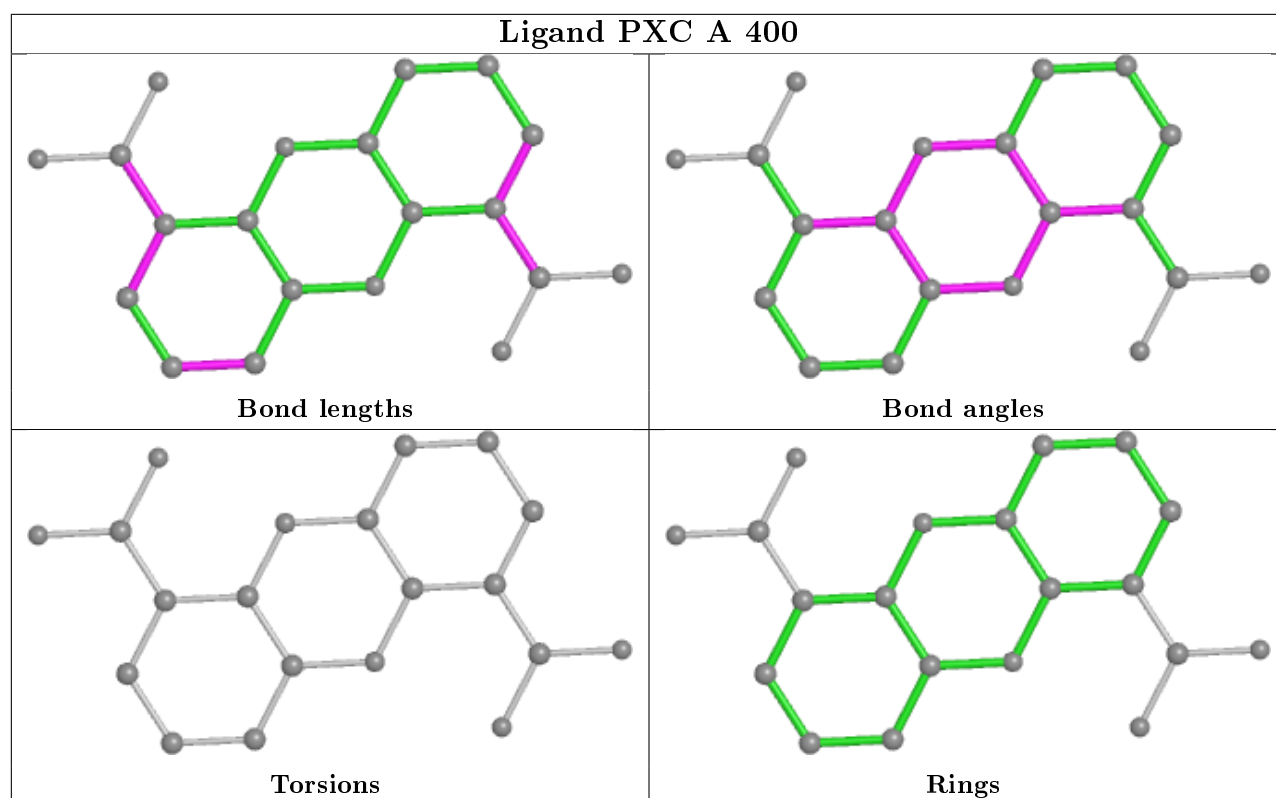
There are no ring outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.18	10 (2%) 53 43	14, 34, 59, 68	0
1	B	352/366 (96%)	-0.24	10 (2%) 53 43	15, 35, 56, 69	3 (0%)
All	All	704/732 (96%)	-0.21	20 (2%) 53 43	14, 34, 57, 69	3 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	THR	3.7
1	A	342	PHE	3.3
1	B	96	SER	3.1
1	A	176	SER	3.0
1	B	103	PRO	2.7
1	A	101	GLY	2.7
1	B	3	ASP	2.6
1	B	354	LYS	2.5
1	A	184	ARG	2.5
1	A	180	THR	2.4
1	B	173	ARG	2.4
1	A	330	ARG	2.4
1	B	102	ALA	2.3
1	B	341	GLY	2.3
1	A	178	GLY	2.3
1	A	29	ARG	2.3
1	B	70	HIS	2.2
1	B	100	THR	2.2
1	A	36	THR	2.2
1	B	215	GLU	2.1

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 monosaccharides in this entry.

6.4 Ligands [i](#)

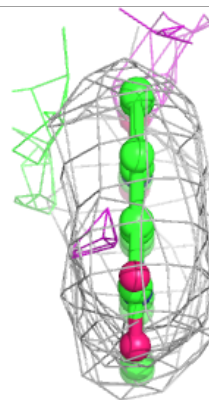
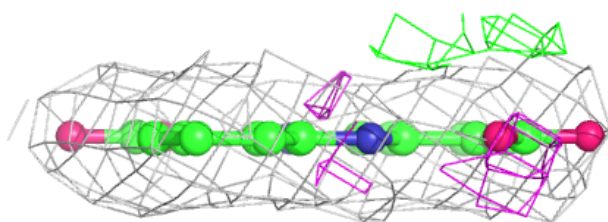
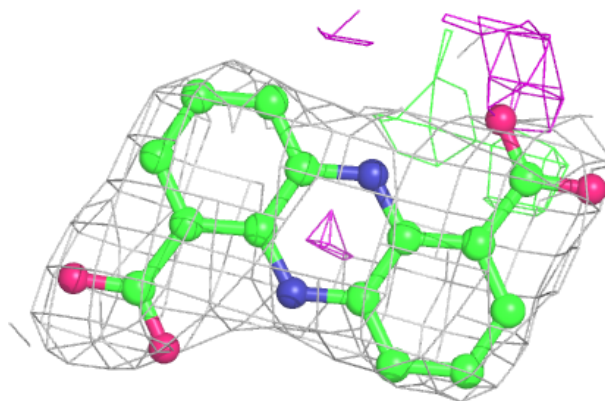
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PXC	B	400	20/20	0.90	0.18	67,68,71,73	0
2	PXC	A	400	20/20	0.94	0.17	44,46,51,55	0

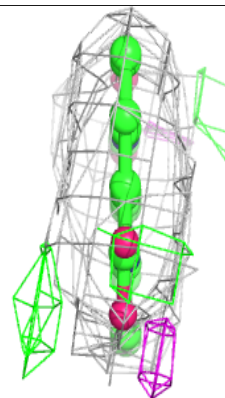
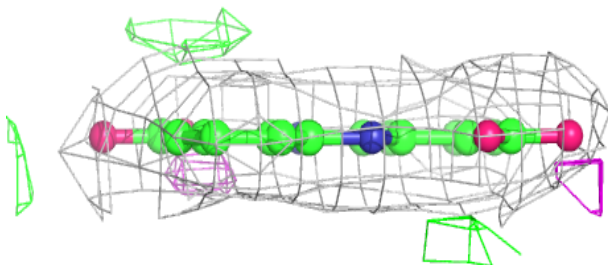
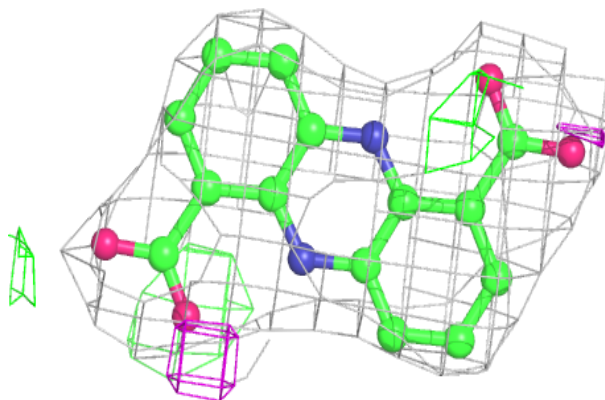
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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