Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 05:23 pm BST

PDB ID	:	3MMP
Title	:	Structure of the Qb replicase, an RNA-dependent RNA polymerase consisting of viral and host proteins
Authors	:	Kidmose, R.T.; Vasiliev, N.N.; Chetverin, A.B.; Knudsen, C.R.; Andersen, G.R.
Deposited on	:	2010-04-20
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.11
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)	:	2.11

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 2.50 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		0.224
Clashscore		9
Ramachandran outliers		0.5%
Sidechain outliers		6.2%
RSRZ outliers		4.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
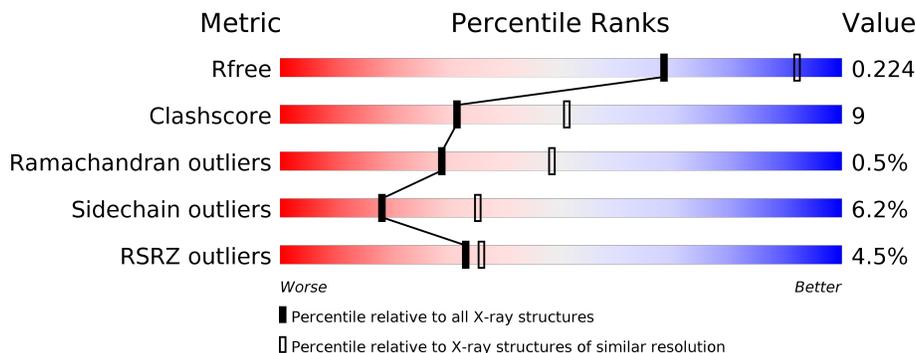
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	678	5% 75% 18% • 5%
1	C	678	7% 75% 17% • 5%
2	F	589	2% 78% 13% • 7%
2	G	589	3% 78% 13% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19419 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 Elongation factor Tu 2, Elongation factor Ts.

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total 4904	C 3095	N 839	O 946	S 24	0	0	0
1	C	643	Total 4904	C 3095	N 839	O 946	S 24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	999	HIS	-	LINKER	UNP P0A6P1
C	999	HIS	-	LINKER	UNP P0A6P1

- Molecule 2 is a protein called RNA-directed RNA polymerase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	549	Total 4318	C 2736	N 757	O 804	S 21	0	0	0
2	F	549	Total 4318	C 2736	N 757	O 804	S 21	0	0	0

- Molecule 3 is (2S)-1-[3-{[(2R)-2-hydroxypropyl]oxy}-2,2-bis({[(2R)-2-hydroxypropyl]oxy}methyl)propoxy]propan-2-ol (three-letter code: PXN) (formula: $C_{17}H_{36}O_8$).
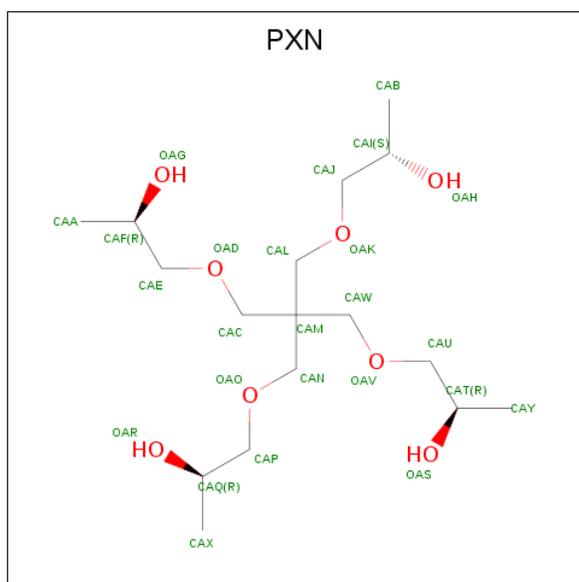
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 25	C 17	O 8	0	0
3	C	1	Total 25	C 17	O 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	171	Total 171	O 171	0	0
4	G	332	Total 332	O 332	0	0
4	C	131	Total 131	O 131	0	0
4	F	291	Total 291	O 291	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: Elongation factor Tu 2, Elongation factor Ts
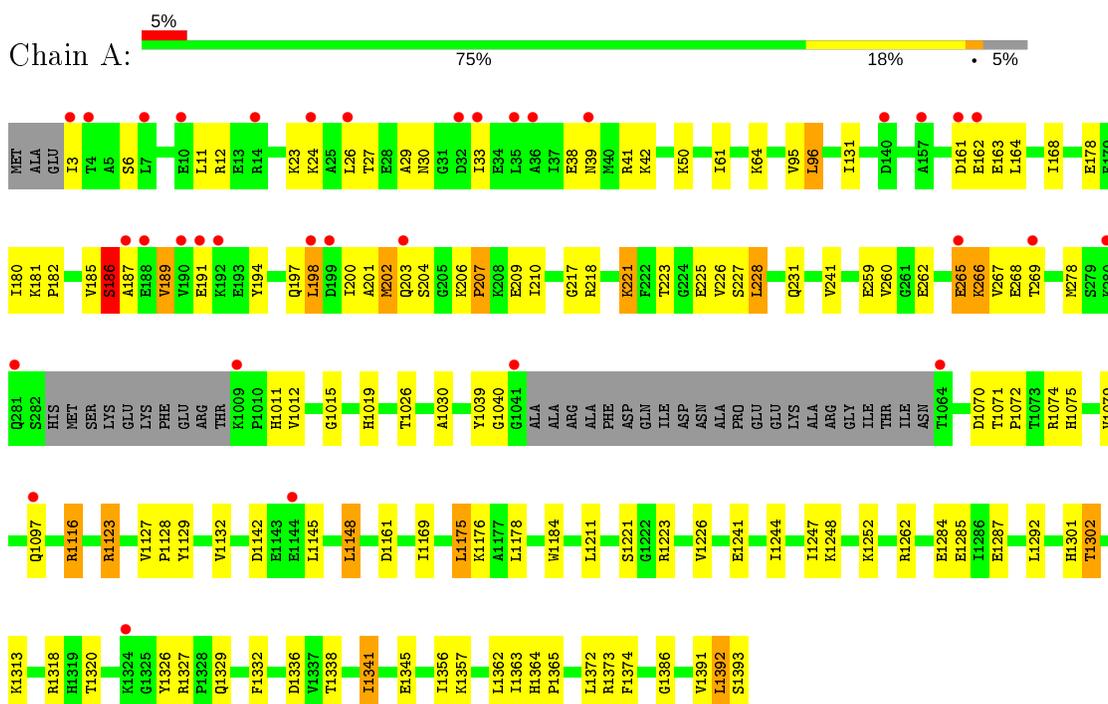
- Molecule 1: Elongation factor Tu 2, Elongation factor Ts
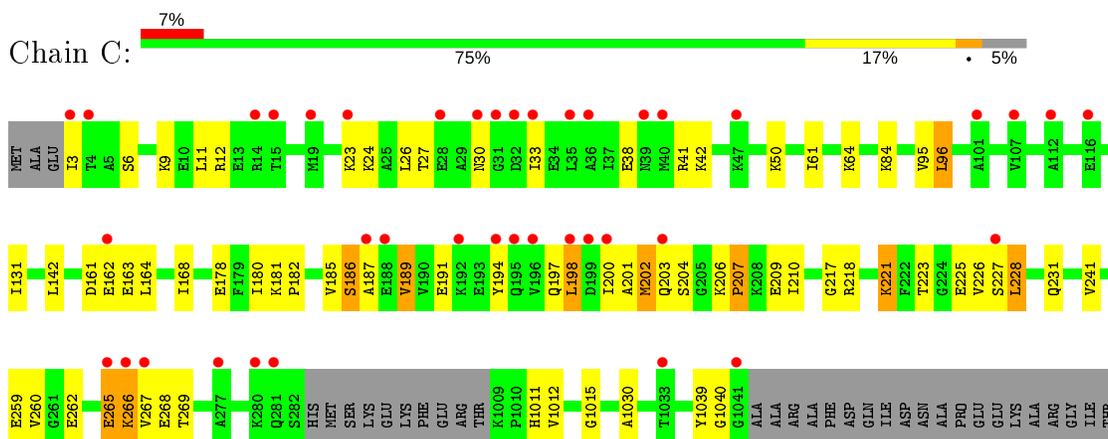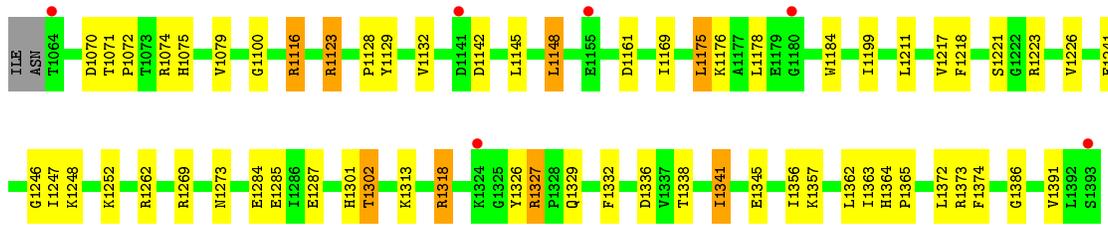
• Molecule 2: RNA-directed RNA polymerase beta chain
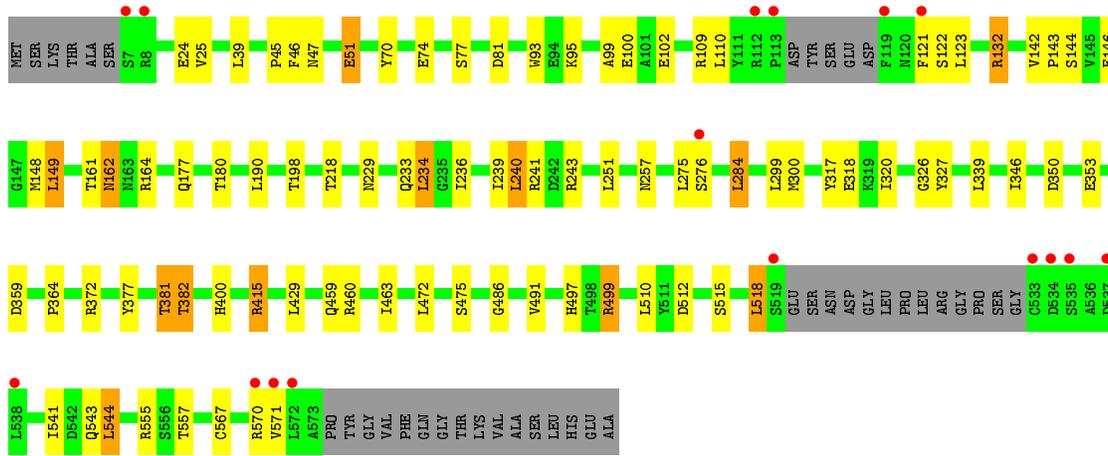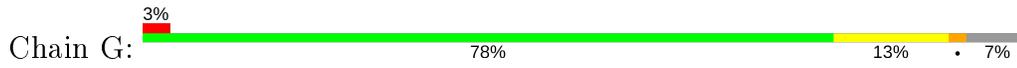
• Molecule 2: RNA-directed RNA polymerase beta chain
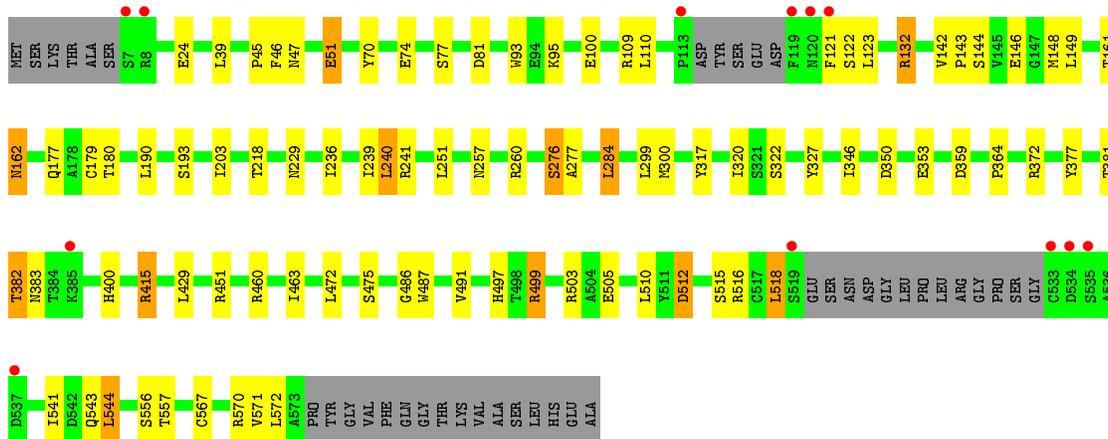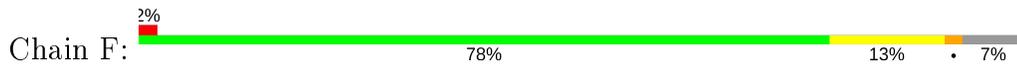
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	254.71Å 139.40Å 101.87Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	47.28 – 2.50 47.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.28-2.50) 99.9 (47.28-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.210 , 0.230 0.205 , 0.224	Depositor DCC
R_{free} test set	1993 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.4	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19419	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: PXN

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	0.33	0/4977	0.55	3/6712 (0.0%)
1	C	0.33	0/4977	0.59	3/6712 (0.0%)
2	F	0.45	0/4412	0.57	0/5980
2	G	0.45	0/4412	0.57	0/5980
All	All	0.39	0/18778	0.57	6/25384 (0.0%)

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	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1318	ARG	NE-CZ-NH2	-16.24	112.18	120.30
1	C	1318	ARG	NE-CZ-NH1	15.90	128.25	120.30
1	A	1318	ARG	NE-CZ-NH2	9.79	125.20	120.30
1	A	1318	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	C	1318	ARG	CD-NE-CZ	7.50	134.10	123.60
1	A	1318	ARG	CD-NE-CZ	5.83	131.76	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1392	LEU	Peptide

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	4904	0	4969	102	0
1	C	4904	0	4969	103	0
2	F	4318	0	4284	76	0
2	G	4318	0	4284	74	0
3	A	25	0	36	4	0
3	C	25	0	36	4	0
4	A	171	0	0	5	0
4	C	131	0	0	2	0
4	F	291	0	0	6	0
4	G	332	0	0	9	0
All	All	19419	0	18578	335	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 9.

All (335) 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)
2:G:121:PHE:CZ	2:F:121:PHE:CZ	2.58	0.92
2:G:499:ARG:HG3	2:G:499:ARG:HH11	1.38	0.88
1:C:64:LYS:HB2	1:C:96:LEU:HD11	1.54	0.88
1:A:64:LYS:HB2	1:A:96:LEU:HD11	1.54	0.87
2:F:499:ARG:HH11	2:F:499:ARG:HG3	1.35	0.87
1:A:1262:ARG:HH22	3:A:1394:PXN:HAAA	1.43	0.83
2:G:148:MET:CE	2:G:236:ILE:HD13	2.11	0.81
1:A:265:GLU:HG3	1:A:266:LYS:H	1.44	0.81
1:C:265:GLU:HG3	1:C:266:LYS:H	1.45	0.80
2:F:570:ARG:HH11	2:F:570:ARG:HG3	1.45	0.80
1:A:1128:PRO:HB2	1:A:1129:TYR:CD2	2.17	0.80
2:F:148:MET:CE	2:F:236:ILE:HD13	2.11	0.79
2:F:180:THR:H	2:F:229:ASN:HD21	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:499:ARG:HG3	2:F:499:ARG:NH1	1.94	0.79
1:C:1128:PRO:HB2	1:C:1129:TYR:CD2	2.18	0.78
2:G:570:ARG:HG3	2:G:570:ARG:HH11	1.46	0.78
2:G:180:THR:H	2:G:229:ASN:HD21	1.31	0.78
2:G:499:ARG:NH1	2:G:499:ARG:HG3	1.96	0.76
1:A:1373:ARG:HG3	1:A:1373:ARG:HH11	1.51	0.76
1:A:1262:ARG:HH22	3:A:1394:PXN:CAA	1.98	0.76
1:C:1123:ARG:HA	1:C:1123:ARG:HE	1.52	0.75
1:A:218:ARG:HD3	4:G:882:HOH:O	1.86	0.75
1:C:1373:ARG:HG3	1:C:1373:ARG:HH11	1.52	0.75
1:A:1123:ARG:HA	1:A:1123:ARG:HE	1.54	0.73
2:G:121:PHE:CE2	2:F:121:PHE:CE2	2.77	0.72
2:F:148:MET:HE3	2:F:236:ILE:HD13	1.70	0.72
1:C:1301:HIS:CE1	1:C:1391:VAL:HG11	2.24	0.71
2:G:148:MET:HE3	2:G:236:ILE:HD13	1.71	0.71
1:A:1011:HIS:CD2	1:A:1075:HIS:HD2	2.10	0.70
1:C:1327:ARG:HG2	2:F:486:GLY:HA3	1.73	0.70
1:C:1273:ASN:HD22	2:F:516:ARG:HH11	1.40	0.70
1:A:207:PRO:HB2	1:A:210:ILE:HG12	1.75	0.68
1:C:1262:ARG:HH22	3:C:1394:PXN:CAA	2.06	0.68
1:C:1248:LYS:HE3	1:C:1285:GLU:O	1.93	0.68
1:C:1011:HIS:CD2	1:C:1075:HIS:HD2	2.11	0.68
1:C:207:PRO:HB2	1:C:210:ILE:HG12	1.75	0.68
1:C:201:ALA:O	1:C:206:LYS:HD3	1.94	0.67
1:A:201:ALA:O	1:A:206:LYS:HD3	1.93	0.67
2:F:132:ARG:HD2	2:F:132:ARG:C	2.14	0.67
2:G:148:MET:HE1	2:G:236:ILE:HD13	1.77	0.66
2:F:148:MET:HE1	2:F:236:ILE:HD13	1.78	0.65
1:A:1248:LYS:HE3	1:A:1285:GLU:O	1.96	0.65
2:G:148:MET:HE2	2:G:239:ILE:HD12	1.78	0.65
2:F:39:LEU:HD21	2:F:45:PRO:HG3	1.79	0.65
2:G:46:PHE:HD1	2:G:51:GLU:HG2	1.63	0.64
2:G:132:ARG:HD2	2:G:132:ARG:C	2.18	0.64
1:C:180:ILE:HG22	1:C:181:LYS:HG3	1.80	0.63
2:F:46:PHE:HD1	2:F:51:GLU:HG2	1.62	0.63
1:A:1301:HIS:CE1	1:A:1391:VAL:HG11	2.33	0.63
2:F:541:ILE:O	2:F:544:LEU:HB2	1.99	0.63
1:C:161:ASP:OD1	1:C:164:LEU:HB2	2.00	0.62
2:G:148:MET:CE	2:G:239:ILE:HD12	2.29	0.62
2:F:95:LYS:NZ	2:F:218:THR:HG21	2.14	0.62
2:F:499:ARG:HH11	2:F:499:ARG:CG	2.10	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:121:PHE:CZ	2:F:121:PHE:CE2	2.88	0.61
1:C:1132:VAL:HB	1:C:1169:ILE:HG12	1.82	0.61
2:F:146:GLU:H	2:F:146:GLU:CD	2.03	0.61
2:G:541:ILE:O	2:G:544:LEU:HB2	2.00	0.61
1:A:161:ASP:OD1	1:A:164:LEU:HB2	2.01	0.61
2:G:95:LYS:NZ	2:G:218:THR:HG21	2.15	0.61
2:G:499:ARG:CG	2:G:499:ARG:HH11	2.12	0.61
1:A:197:GLN:HA	1:A:200:ILE:HD12	1.82	0.60
2:F:497:HIS:HD2	2:F:557:THR:OG1	1.84	0.60
1:A:1313:LYS:HD2	2:G:571:VAL:HG21	1.83	0.60
2:G:372:ARG:HD3	4:G:776:HOH:O	2.01	0.60
1:A:180:ILE:HG22	1:A:181:LYS:HG3	1.82	0.60
2:F:132:ARG:HD2	2:F:132:ARG:O	2.01	0.60
1:A:1097:GLN:HA	4:A:1397:HOH:O	2.00	0.59
1:A:1326:TYR:HB3	1:A:1341:ILE:CD1	2.32	0.59
2:G:497:HIS:HD2	2:G:557:THR:OG1	1.84	0.59
1:C:1247:ILE:HG21	1:C:1287:GLU:OE2	2.03	0.59
1:C:84:LYS:HD3	4:C:927:HOH:O	2.01	0.59
1:A:228:LEU:HD22	1:A:241:VAL:HG11	1.84	0.59
1:C:197:GLN:HA	1:C:200:ILE:HD12	1.85	0.58
2:F:148:MET:HE2	2:F:239:ILE:HD12	1.84	0.58
2:G:39:LEU:HD21	2:G:45:PRO:HG3	1.85	0.58
2:G:132:ARG:HD2	2:G:132:ARG:O	2.04	0.58
1:A:1373:ARG:CG	1:A:1373:ARG:HH11	2.16	0.58
1:A:182:PRO:HB3	1:A:223:THR:HG22	1.86	0.58
1:C:38:GLU:HG3	1:C:42:LYS:NZ	2.19	0.58
1:C:259:GLU:HB3	1:C:262:GLU:HG3	1.86	0.57
1:C:1326:TYR:HB3	1:C:1341:ILE:CD1	2.34	0.57
1:A:1329:GLN:HE21	1:A:1336:ASP:HB3	1.69	0.57
1:A:1247:ILE:HG21	1:A:1287:GLU:OE2	2.05	0.57
1:A:38:GLU:HG3	1:A:42:LYS:NZ	2.19	0.57
2:F:148:MET:CE	2:F:239:ILE:HD12	2.35	0.56
2:G:146:GLU:CD	2:G:146:GLU:H	2.08	0.56
2:G:243:ARG:HD2	4:G:645:HOH:O	2.05	0.56
1:A:1123:ARG:HH11	1:A:1161:ASP:HB2	1.70	0.56
1:A:1132:VAL:HB	1:A:1169:ILE:HG12	1.87	0.56
1:C:1373:ARG:CG	1:C:1373:ARG:HH11	2.17	0.56
1:C:9:LYS:HB2	1:C:1148:LEU:HD21	1.87	0.56
2:F:162:ASN:HD22	2:F:162:ASN:N	2.03	0.56
1:C:1123:ARG:HH11	1:C:1161:ASP:HB2	1.71	0.55
1:C:1326:TYR:HB3	1:C:1341:ILE:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:353:GLU:HG2	2:F:364:PRO:HG3	1.88	0.55
2:G:234:LEU:HD13	2:G:326:GLY:HA3	1.88	0.55
2:G:353:GLU:HG2	2:G:364:PRO:HG3	1.87	0.55
1:A:1326:TYR:HB3	1:A:1341:ILE:HD13	1.89	0.55
2:G:243:ARG:CD	4:G:645:HOH:O	2.55	0.55
2:G:46:PHE:HD1	2:G:51:GLU:CG	2.20	0.55
2:F:46:PHE:HD1	2:F:51:GLU:CG	2.19	0.54
1:A:265:GLU:HG3	1:A:266:LYS:N	2.20	0.54
1:A:259:GLU:HB3	1:A:262:GLU:HG3	1.88	0.54
1:C:1142:ASP:HB3	1:C:1145:LEU:HG	1.89	0.54
1:C:182:PRO:HB3	1:C:223:THR:HG22	1.90	0.54
1:C:228:LEU:HD22	1:C:241:VAL:HG11	1.88	0.54
2:F:148:MET:HE3	2:F:236:ILE:CD1	2.36	0.54
1:A:1123:ARG:NH1	1:A:1161:ASP:HB2	2.23	0.54
1:C:1262:ARG:HH22	3:C:1394:PXN:HAA	1.71	0.54
1:C:204:SER:HB2	1:C:206:LYS:HG2	1.91	0.53
2:F:142:VAL:HG22	2:F:143:PRO:HD2	1.90	0.53
1:A:1011:HIS:HD2	1:A:1075:HIS:HD2	1.55	0.53
1:C:1123:ARG:NH1	1:C:1161:ASP:HB2	2.23	0.53
2:F:300:MET:CE	2:F:320:ILE:HD12	2.39	0.53
2:G:81:ASP:OD2	2:G:415:ARG:HD3	2.08	0.53
1:C:1329:GLN:HE21	1:C:1336:ASP:HB3	1.74	0.53
2:F:100:GLU:OE2	2:F:317:TYR:HA	2.09	0.53
1:C:1176:LYS:HB3	1:C:1184:TRP:CD1	2.44	0.53
2:G:162:ASN:HD22	2:G:162:ASN:N	2.07	0.53
1:A:221:LYS:O	1:A:225:GLU:HG3	2.09	0.52
1:C:1128:PRO:HB2	1:C:1129:TYR:CE2	2.44	0.52
1:A:1142:ASP:HB3	1:A:1145:LEU:HG	1.90	0.52
2:G:148:MET:HE2	2:G:239:ILE:CD1	2.38	0.52
2:F:372:ARG:HG2	2:F:382:THR:HG21	1.91	0.52
2:G:100:GLU:OE2	2:G:317:TYR:HA	2.10	0.52
2:G:300:MET:CE	2:G:320:ILE:HD12	2.40	0.52
1:A:1320:THR:HB	4:A:1416:HOH:O	2.10	0.52
2:G:142:VAL:HG22	2:G:143:PRO:HD2	1.92	0.52
2:G:121:PHE:CE2	2:F:121:PHE:CZ	2.98	0.52
1:C:1262:ARG:HH22	3:C:1394:PXN:HAAA	1.75	0.52
2:G:459:GLN:NE2	4:G:872:HOH:O	2.44	0.51
1:C:1011:HIS:HD2	1:C:1075:HIS:HD2	1.54	0.51
2:G:463:ILE:HG22	2:G:491:VAL:HG11	1.93	0.51
1:A:1128:PRO:HB2	1:A:1129:TYR:CE2	2.45	0.51
2:F:570:ARG:NH1	2:F:570:ARG:HG3	2.21	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:SER:O	1:C:231:GLN:HG3	2.10	0.51
2:G:93:TRP:HA	2:G:93:TRP:CE3	2.46	0.51
1:A:200:ILE:O	1:A:203:GLN:HG2	2.11	0.51
1:A:164:LEU:O	1:A:168:ILE:HG12	2.11	0.51
1:C:38:GLU:HG3	1:C:42:LYS:HZ2	1.75	0.51
2:G:148:MET:HE3	2:G:236:ILE:CD1	2.39	0.51
1:C:221:LYS:O	1:C:225:GLU:HG3	2.11	0.51
2:F:350:ASP:O	2:F:353:GLU:HB2	2.11	0.51
1:A:204:SER:HB2	1:A:206:LYS:HG2	1.93	0.51
1:C:198:LEU:O	1:C:202:MET:HB2	2.11	0.50
2:G:121:PHE:HZ	2:F:121:PHE:CZ	2.23	0.50
2:G:518:LEU:HD12	2:G:518:LEU:C	2.31	0.50
2:F:518:LEU:C	2:F:518:LEU:HD12	2.32	0.50
2:G:518:LEU:HD22	4:G:717:HOH:O	2.11	0.50
1:C:204:SER:HB2	1:C:206:LYS:HD2	1.94	0.50
1:C:265:GLU:HG3	1:C:266:LYS:N	2.20	0.50
1:A:1176:LYS:HB3	1:A:1184:TRP:CD1	2.47	0.50
1:A:185:VAL:O	1:A:187:ALA:N	2.45	0.50
1:A:204:SER:HB2	1:A:206:LYS:HD2	1.93	0.50
1:C:217:GLY:O	1:C:221:LYS:HD2	2.12	0.50
2:F:556:SER:HB2	4:F:677:HOH:O	2.12	0.50
1:A:1338:THR:HB	1:A:1363:ILE:CD1	2.41	0.50
1:A:198:LEU:C	1:A:198:LEU:HD12	2.32	0.50
1:C:164:LEU:O	1:C:168:ILE:HG12	2.12	0.50
1:C:200:ILE:O	1:C:203:GLN:HG2	2.12	0.50
1:C:198:LEU:HD12	1:C:198:LEU:C	2.33	0.49
1:C:1338:THR:O	1:C:1363:ILE:HG13	2.13	0.49
1:C:1030:ALA:HA	1:C:1178:LEU:HD13	1.94	0.49
2:F:161:THR:C	2:F:162:ASN:HD22	2.16	0.49
2:G:350:ASP:O	2:G:353:GLU:HB2	2.13	0.49
1:A:217:GLY:O	1:A:221:LYS:HD2	2.12	0.49
1:A:186:SER:O	1:A:189:VAL:HG12	2.12	0.49
1:A:198:LEU:O	1:A:202:MET:HB2	2.12	0.49
1:A:227:SER:O	1:A:231:GLN:HG3	2.12	0.49
2:G:515:SER:O	2:G:518:LEU:HG	2.13	0.49
2:F:463:ILE:HG22	2:F:491:VAL:HG11	1.95	0.49
2:F:93:TRP:CE3	2:F:93:TRP:HA	2.47	0.49
1:A:1030:ALA:HA	1:A:1178:LEU:HD13	1.93	0.49
2:F:144:SER:HB2	2:F:146:GLU:OE1	2.13	0.49
1:A:218:ARG:HH11	1:A:218:ARG:HG2	1.77	0.48
1:C:185:VAL:O	1:C:187:ALA:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ARG:HH11	1:C:218:ARG:HG2	1.77	0.48
2:G:161:THR:C	2:G:162:ASN:HD22	2.16	0.48
1:A:1332:PHE:HD1	1:A:1372:LEU:HD11	1.78	0.48
1:A:3:ILE:HD12	1:A:26:LEU:HB3	1.96	0.48
2:F:95:LYS:HZ2	2:F:218:THR:HG21	1.78	0.48
1:A:1019:HIS:HD2	4:A:626:HOH:O	1.97	0.48
2:F:162:ASN:ND2	2:F:177:GLN:HE22	2.12	0.48
2:G:570:ARG:CG	2:G:570:ARG:HH11	2.19	0.48
1:C:3:ILE:HD12	1:C:26:LEU:HB3	1.96	0.48
2:F:81:ASP:OD2	2:F:415:ARG:HD3	2.13	0.48
1:C:1332:PHE:HD1	1:C:1372:LEU:HD11	1.78	0.48
1:C:191:GLU:O	1:C:191:GLU:HG2	2.14	0.48
2:G:95:LYS:HZ2	2:G:218:THR:HG21	1.78	0.48
2:G:229:ASN:O	2:G:233:GLN:HG3	2.14	0.48
2:G:74:GLU:HA	2:G:77:SER:OG	2.14	0.48
1:C:1262:ARG:NH1	2:F:193:SER:OG	2.46	0.47
2:F:570:ARG:HH11	2:F:570:ARG:CG	2.18	0.47
2:G:570:ARG:HG3	2:G:570:ARG:NH1	2.22	0.47
1:C:1284:GLU:H	1:C:1284:GLU:CD	2.18	0.47
1:C:3:ILE:HG21	1:C:23:LYS:HD2	1.96	0.47
2:F:451:ARG:NH2	4:F:679:HOH:O	2.46	0.47
1:C:267:VAL:HG13	1:C:267:VAL:O	2.15	0.47
1:A:1071:THR:HB	1:A:1072:PRO:HD2	1.97	0.47
1:C:1313:LYS:HD2	2:F:571:VAL:HG21	1.95	0.47
1:A:191:GLU:O	1:A:191:GLU:HG2	2.14	0.47
1:C:186:SER:O	1:C:189:VAL:HG12	2.14	0.47
1:A:1373:ARG:CG	1:A:1373:ARG:NH1	2.76	0.47
1:C:1373:ARG:NH1	1:C:1373:ARG:CG	2.77	0.47
1:A:267:VAL:O	1:A:267:VAL:HG13	2.14	0.47
2:F:515:SER:O	2:F:518:LEU:HG	2.15	0.47
2:G:100:GLU:OE2	2:G:318:GLU:N	2.35	0.47
2:G:555:ARG:HB3	2:G:555:ARG:HE	1.55	0.47
1:C:1356:ILE:HG12	1:C:1357:LYS:N	2.30	0.47
1:A:3:ILE:HG21	1:A:23:LYS:HD2	1.96	0.46
2:G:144:SER:HB2	2:G:146:GLU:OE1	2.14	0.46
1:A:1284:GLU:CD	1:A:1284:GLU:H	2.18	0.46
2:F:100:GLU:HG2	4:F:776:HOH:O	2.16	0.46
1:A:3:ILE:HD11	1:A:26:LEU:O	2.15	0.46
1:C:1318:ARG:NH2	2:F:487:TRP:O	2.46	0.46
2:G:372:ARG:HG2	2:G:382:THR:HG21	1.96	0.46
1:C:1071:THR:HB	1:C:1072:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1262:ARG:NH1	2:F:193:SER:CB	2.79	0.46
1:A:1356:ILE:HG12	1:A:1357:LYS:N	2.30	0.46
1:A:1392:LEU:O	1:A:1393:SER:C	2.54	0.46
1:A:265:GLU:O	1:A:266:LYS:HB2	2.16	0.46
1:C:11:LEU:HD22	1:C:26:LEU:HG	1.97	0.46
3:A:1394:PXN:HAWA	3:A:1394:PXN:HAT	1.64	0.45
1:C:265:GLU:O	1:C:266:LYS:HB2	2.16	0.45
2:F:74:GLU:HA	2:F:77:SER:OG	2.16	0.45
2:G:123:LEU:N	2:F:121:PHE:CE2	2.84	0.45
1:A:11:LEU:HD22	1:A:26:LEU:HG	1.97	0.45
1:C:1338:THR:HB	1:C:1363:ILE:CD1	2.47	0.45
1:C:1116:ARG:HE	1:C:1116:ARG:HB3	1.44	0.45
1:A:1327:ARG:HG2	2:G:486:GLY:HA3	1.99	0.45
1:A:61:ILE:HG12	1:A:260:VAL:HG23	1.98	0.45
1:A:1241:GLU:OE2	1:A:1252:LYS:HE2	2.17	0.45
1:C:61:ILE:HG12	1:C:260:VAL:HG23	1.98	0.45
1:A:178:GLU:HB2	1:A:226:VAL:CG1	2.47	0.45
1:C:1241:GLU:OE2	1:C:1252:LYS:HE2	2.17	0.44
1:C:1332:PHE:HD1	1:C:1372:LEU:CD1	2.30	0.44
2:F:148:MET:HE2	2:F:239:ILE:CD1	2.46	0.44
2:G:240:LEU:HD12	2:G:240:LEU:HA	1.86	0.44
1:A:1302:THR:HG22	1:A:1362:LEU:O	2.17	0.44
1:C:206:LYS:H	1:C:206:LYS:HG2	1.51	0.44
1:C:3:ILE:HD11	1:C:26:LEU:O	2.17	0.44
2:F:284:LEU:CD1	2:F:320:ILE:HA	2.48	0.44
2:G:99:ALA:HB3	4:G:678:HOH:O	2.17	0.44
1:C:1217:VAL:O	2:F:503:ARG:NH2	2.51	0.44
1:C:1374:PHE:CZ	1:C:1386:GLY:HA3	2.53	0.44
1:C:1218:PHE:HA	2:F:505:GLU:OE2	2.18	0.44
1:C:1273:ASN:HB3	2:F:516:ARG:HG3	1.99	0.44
2:G:284:LEU:CD1	2:G:320:ILE:HA	2.47	0.44
1:A:1374:PHE:CZ	1:A:1386:GLY:HA3	2.53	0.43
2:G:570:ARG:CG	2:G:570:ARG:NH1	2.78	0.43
2:F:240:LEU:HA	2:F:240:LEU:HD12	1.84	0.43
2:G:132:ARG:HD3	4:G:740:HOH:O	2.19	0.43
2:G:162:ASN:ND2	2:G:177:GLN:HE22	2.16	0.43
1:A:265:GLU:CG	1:A:266:LYS:H	2.24	0.43
1:A:1326:TYR:HB3	1:A:1341:ILE:HD11	2.00	0.43
1:A:265:GLU:O	1:A:266:LYS:CB	2.67	0.43
1:C:1011:HIS:CD2	1:C:1075:HIS:CD2	2.99	0.43
1:A:1011:HIS:CD2	1:A:1075:HIS:CD2	2.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:SER:HB2	1:A:206:LYS:CD	2.49	0.43
1:C:1100:GLY:HA3	1:C:1199:ILE:HD13	2.00	0.43
1:C:178:GLU:HB2	1:C:226:VAL:CG1	2.49	0.43
2:G:121:PHE:CE2	2:F:123:LEU:N	2.86	0.43
1:C:95:VAL:HG11	1:C:131:ILE:HD13	2.00	0.43
1:C:226:VAL:HG12	1:C:226:VAL:O	2.18	0.43
1:A:268:GLU:HG2	1:A:269:THR:N	2.34	0.43
1:C:268:GLU:HG2	1:C:269:THR:N	2.34	0.43
2:F:570:ARG:NH1	2:F:570:ARG:CG	2.77	0.43
2:G:241:ARG:HG3	2:G:251:LEU:HB2	2.00	0.43
1:A:194:TYR:CE2	1:A:198:LEU:HD23	2.54	0.43
2:G:109:ARG:NH1	2:G:377:TYR:O	2.51	0.43
1:C:265:GLU:O	1:C:266:LYS:CB	2.67	0.42
2:F:241:ARG:HG3	2:F:251:LEU:HB2	2.00	0.42
2:F:571:VAL:HG12	2:F:572:LEU:O	2.19	0.42
2:F:260:ARG:HG2	4:F:770:HOH:O	2.19	0.42
2:G:121:PHE:CZ	2:F:121:PHE:HZ	2.30	0.42
2:G:70:TYR:OH	2:G:400:HIS:HD2	2.02	0.42
1:A:1012:VAL:HG21	1:A:1074:ARG:HD3	2.00	0.42
1:A:38:GLU:HG3	1:A:42:LYS:HZ2	1.83	0.42
1:C:1364:HIS:HB2	1:C:1365:PRO:CD	2.49	0.42
3:C:1394:PXN:HAT	3:C:1394:PXN:HAWA	1.82	0.42
1:C:1175:LEU:HA	1:C:1175:LEU:HD13	1.83	0.42
1:C:1262:ARG:NH1	2:F:193:SER:HB2	2.33	0.42
1:A:278:MET:HE2	1:A:1026:THR:HG23	2.02	0.42
1:C:1364:HIS:HD2	4:C:676:HOH:O	2.02	0.42
1:A:1332:PHE:HD1	1:A:1372:LEU:CD1	2.32	0.42
1:A:95:VAL:HG11	1:A:131:ILE:HD13	2.01	0.42
2:G:381:THR:O	2:G:381:THR:CG2	2.67	0.42
1:A:1175:LEU:HA	1:A:1175:LEU:HD13	1.85	0.42
1:C:1148:LEU:HA	1:C:1148:LEU:HD12	1.70	0.42
1:C:24:LYS:O	1:C:27:THR:HB	2.20	0.42
2:F:277:ALA:HB2	4:F:832:HOH:O	2.20	0.42
1:A:1127:VAL:HA	1:A:1128:PRO:HD3	1.91	0.42
1:A:24:LYS:O	1:A:27:THR:HB	2.20	0.42
2:G:99:ALA:O	2:G:102:GLU:HB3	2.20	0.42
1:A:1338:THR:O	1:A:1363:ILE:HG13	2.19	0.42
1:A:38:GLU:HG3	1:A:42:LYS:HZ1	1.83	0.42
1:A:1039:TYR:HA	1:C:1039:TYR:HA	2.02	0.41
1:A:1364:HIS:HB2	1:A:1365:PRO:CD	2.50	0.41
1:C:1015:GLY:HA2	1:C:1079:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:SER:HB2	1:C:206:LYS:CD	2.49	0.41
2:F:146:GLU:N	2:F:146:GLU:CD	2.73	0.41
1:C:1273:ASN:HB3	2:F:516:ARG:HD3	2.01	0.41
2:F:179:CYS:O	2:F:203:ILE:HA	2.20	0.41
1:A:218:ARG:NH1	1:A:218:ARG:HG2	2.35	0.41
1:A:178:GLU:HB2	1:A:226:VAL:HG13	2.03	0.41
1:C:142:LEU:HA	1:C:142:LEU:HD23	1.92	0.41
1:C:194:TYR:CE2	1:C:198:LEU:HD23	2.55	0.41
2:F:100:GLU:CG	4:F:776:HOH:O	2.68	0.41
2:F:512:ASP:OD1	2:F:512:ASP:C	2.59	0.41
1:A:1019:HIS:CD2	4:A:626:HOH:O	2.72	0.41
1:A:1148:LEU:HD12	1:A:1148:LEU:HA	1.69	0.41
1:A:1015:GLY:HA2	1:A:1079:VAL:O	2.20	0.41
1:A:226:VAL:HG12	1:A:226:VAL:O	2.20	0.41
2:G:164:ARG:H	2:G:164:ARG:HG2	1.60	0.41
1:C:1302:THR:HG22	1:C:1362:LEU:O	2.21	0.41
1:C:218:ARG:NH1	1:C:218:ARG:HG2	2.35	0.41
2:F:70:TYR:OH	2:F:400:HIS:HD2	2.03	0.41
2:G:149:LEU:HD12	2:G:149:LEU:HA	1.98	0.41
1:A:206:LYS:H	1:A:206:LYS:HG2	1.50	0.41
1:C:1012:VAL:HG21	1:C:1074:ARG:HD3	2.01	0.41
1:C:38:GLU:OE1	1:C:38:GLU:HA	2.21	0.41
1:A:1116:ARG:HE	1:A:1116:ARG:HB3	1.45	0.41
1:A:1176:LYS:HD2	1:A:1176:LYS:HA	1.81	0.41
1:A:1244:ILE:HD13	1:A:1292:LEU:CD2	2.51	0.41
2:G:164:ARG:HG2	4:G:753:HOH:O	2.21	0.41
2:G:275:LEU:HA	2:G:275:LEU:HD23	1.92	0.40
1:A:1338:THR:HB	1:A:1363:ILE:HD12	2.03	0.40
2:F:276:SER:HB2	2:F:383:ASN:HB2	2.03	0.40
1:A:29:ALA:HB2	1:A:39:ASN:ND2	2.37	0.40
1:C:1176:LYS:HB3	1:C:1184:TRP:CG	2.56	0.40
2:F:109:ARG:NH1	2:F:377:TYR:O	2.54	0.40
1:A:1262:ARG:NH2	2:G:149:LEU:HD11	2.37	0.40
3:A:1394:PXN:HAXA	4:A:741:HOH:O	2.22	0.40
1:C:1246:GLY:O	1:C:1248:LYS:N	2.53	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	637/678 (94%)	608 (95%)	24 (4%)	5 (1%)	19	35
1	C	637/678 (94%)	610 (96%)	22 (4%)	5 (1%)	19	35
2	F	543/589 (92%)	536 (99%)	6 (1%)	1 (0%)	47	68
2	G	543/589 (92%)	536 (99%)	6 (1%)	1 (0%)	47	68
All	All	2360/2534 (93%)	2290 (97%)	58 (2%)	12 (0%)	29	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	GLU
2	G	276	SER
1	C	265	GLU
2	F	276	SER
1	A	186	SER
1	A	266	LYS
1	A	1040	GLY
1	C	186	SER
1	C	266	LYS
1	C	1040	GLY
1	C	207	PRO
1	A	207	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	520/548 (95%)	492 (95%)	28 (5%)	22	42
1	C	520/548 (95%)	491 (94%)	29 (6%)	21	40
2	F	471/503 (94%)	440 (93%)	31 (7%)	16	32
2	G	471/503 (94%)	437 (93%)	34 (7%)	14	28
All	All	1982/2102 (94%)	1860 (94%)	122 (6%)	18	35

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	12	ARG
1	A	30	ASN
1	A	33	ILE
1	A	41	ARG
1	A	50	LYS
1	A	96	LEU
1	A	162	GLU
1	A	163	GLU
1	A	186	SER
1	A	189	VAL
1	A	198	LEU
1	A	202	MET
1	A	209	GLU
1	A	221	LYS
1	A	228	LEU
1	A	1070	ASP
1	A	1116	ARG
1	A	1123	ARG
1	A	1148	LEU
1	A	1175	LEU
1	A	1211	LEU
1	A	1221	SER
1	A	1223	ARG
1	A	1226	VAL
1	A	1302	THR
1	A	1341	ILE
1	A	1345	GLU
2	G	24	GLU
2	G	25	VAL
2	G	47	ASN
2	G	51	GLU
2	G	110	LEU

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Mol	Chain	Res	Type
2	G	122	SER
2	G	132	ARG
2	G	149	LEU
2	G	162	ASN
2	G	190	LEU
2	G	198	THR
2	G	234	LEU
2	G	240	LEU
2	G	257	ASN
2	G	284	LEU
2	G	299	LEU
2	G	327	TYR
2	G	339	LEU
2	G	346	ILE
2	G	359	ASP
2	G	381	THR
2	G	382	THR
2	G	415	ARG
2	G	429	LEU
2	G	460	ARG
2	G	472	LEU
2	G	475	SER
2	G	499	ARG
2	G	510	LEU
2	G	512	ASP
2	G	518	LEU
2	G	543	GLN
2	G	544	LEU
2	G	567	CYS
1	C	6	SER
1	C	12	ARG
1	C	30	ASN
1	C	33	ILE
1	C	41	ARG
1	C	50	LYS
1	C	96	LEU
1	C	162	GLU
1	C	163	GLU
1	C	189	VAL
1	C	198	LEU
1	C	202	MET
1	C	209	GLU

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Mol	Chain	Res	Type
1	C	221	LYS
1	C	228	LEU
1	C	1070	ASP
1	C	1116	ARG
1	C	1123	ARG
1	C	1148	LEU
1	C	1175	LEU
1	C	1211	LEU
1	C	1221	SER
1	C	1223	ARG
1	C	1226	VAL
1	C	1269	ARG
1	C	1302	THR
1	C	1327	ARG
1	C	1341	ILE
1	C	1345	GLU
2	F	24	GLU
2	F	47	ASN
2	F	51	GLU
2	F	110	LEU
2	F	122	SER
2	F	132	ARG
2	F	149	LEU
2	F	162	ASN
2	F	190	LEU
2	F	240	LEU
2	F	257	ASN
2	F	284	LEU
2	F	299	LEU
2	F	322	SER
2	F	327	TYR
2	F	346	ILE
2	F	359	ASP
2	F	381	THR
2	F	382	THR
2	F	415	ARG
2	F	429	LEU
2	F	460	ARG
2	F	472	LEU
2	F	475	SER
2	F	499	ARG
2	F	510	LEU

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Mol	Chain	Res	Type
2	F	512	ASP
2	F	518	LEU
2	F	543	GLN
2	F	544	LEU
2	F	567	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	146	GLN
1	A	197	GLN
1	A	203	GLN
1	A	249	ASN
1	A	1011	HIS
1	A	1013	ASN
1	A	1019	HIS
1	A	1075	HIS
1	A	1273	ASN
1	A	1329	GLN
2	G	162	ASN
2	G	229	ASN
2	G	257	ASN
2	G	269	ASN
2	G	400	HIS
2	G	459	GLN
2	G	497	HIS
1	C	113	GLN
1	C	146	GLN
1	C	197	GLN
1	C	203	GLN
1	C	249	ASN
1	C	1011	HIS
1	C	1013	ASN
1	C	1019	HIS
1	C	1075	HIS
1	C	1251	GLN
1	C	1273	ASN
1	C	1329	GLN
2	F	162	ASN
2	F	229	ASN
2	F	257	ASN

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Mol	Chain	Res	Type
2	F	269	ASN
2	F	400	HIS
2	F	459	GLN
2	F	497	HIS

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 carbohydrates 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	#$|Z| > 2$
3	PXN	A	1394	-	20,24,24	0.71	0	22,30,30	1.81	7 (31%)
3	PXN	C	1394	-	20,24,24	0.56	0	22,30,30	2.03	11 (50%)

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
3	PXN	A	1394	-	-	14/28/28/28	-
3	PXN	C	1394	-	-	13/28/28/28	-

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1394	PXN	OAV-CAW-CAM	4.24	120.41	108.76
3	A	1394	PXN	OAV-CAW-CAM	3.32	117.88	108.76
3	A	1394	PXN	OAK-CAL-CAM	3.21	117.57	108.76
3	C	1394	PXN	OAD-CAC-CAM	3.08	117.23	108.76
3	C	1394	PXN	OAK-CAL-CAM	3.03	117.08	108.76
3	A	1394	PXN	OAD-CAC-CAM	2.93	116.80	108.76
3	C	1394	PXN	OAO-CAN-CAM	2.85	116.59	108.76
3	C	1394	PXN	OAV-CAU-CAT	2.59	118.35	109.26
3	C	1394	PXN	CAC-OAD-CAE	2.57	121.03	113.08
3	C	1394	PXN	CAL-OAK-CAJ	2.40	120.49	113.08
3	C	1394	PXN	OAO-CAP-CAQ	2.38	117.61	109.26
3	A	1394	PXN	OAV-CAU-CAT	2.33	117.43	109.26
3	C	1394	PXN	CAN-OAO-CAP	2.26	120.06	113.08
3	A	1394	PXN	OAO-CAN-CAM	2.22	114.87	108.76
3	C	1394	PXN	OAD-CAE-CAF	2.22	117.06	109.26
3	A	1394	PXN	OAK-CAJ-CAI	2.15	116.80	109.26
3	A	1394	PXN	OAD-CAE-CAF	2.06	116.49	109.26
3	C	1394	PXN	OAK-CAJ-CAI	2.06	116.49	109.26

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1394	PXN	OAD-CAE-CAF-CAA
3	A	1394	PXN	CAT-CAU-OAV-CAW
3	C	1394	PXN	OAD-CAE-CAF-CAA
3	C	1394	PXN	CAT-CAU-OAV-CAW
3	A	1394	PXN	CAL-CAM-CAW-OAV
3	C	1394	PXN	CAC-CAM-CAW-OAV
3	C	1394	PXN	CAL-CAM-CAW-OAV
3	A	1394	PXN	CAC-CAM-CAW-OAV
3	A	1394	PXN	CAN-CAM-CAW-OAV
3	C	1394	PXN	CAN-CAM-CAW-OAV
3	C	1394	PXN	OAD-CAE-CAF-OAG
3	C	1394	PXN	OAO-CAP-CAQ-OAR

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Mol	Chain	Res	Type	Atoms
3	A	1394	PXN	CAQ-CAP-OAO-CAN
3	C	1394	PXN	CAB-CAI-CAJ-OAK
3	A	1394	PXN	CAM-CAL-OAK-CAJ
3	A	1394	PXN	CAM-CAW-OAV-CAU
3	C	1394	PXN	CAM-CAL-OAK-CAJ
3	A	1394	PXN	OAD-CAE-CAF-OAG
3	C	1394	PXN	CAQ-CAP-OAO-CAN
3	A	1394	PXN	OAK-CAL-CAM-CAC
3	C	1394	PXN	OAS-CAT-CAU-OAV
3	A	1394	PXN	OAK-CAL-CAM-CAW
3	A	1394	PXN	OAS-CAT-CAU-OAV
3	A	1394	PXN	OAK-CAL-CAM-CAN
3	A	1394	PXN	CAF-CAE-OAD-CAC
3	C	1394	PXN	CAF-CAE-OAD-CAC
3	C	1394	PXN	OAH-CAI-CAJ-OAK

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1394	PXN	4	0
3	C	1394	PXN	4	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 PXN A 1394

Bond lengths

Bond angles

Torsions

Rings

Ligand PXN C 1394

Bond lengths

Bond angles

Torsions

Rings
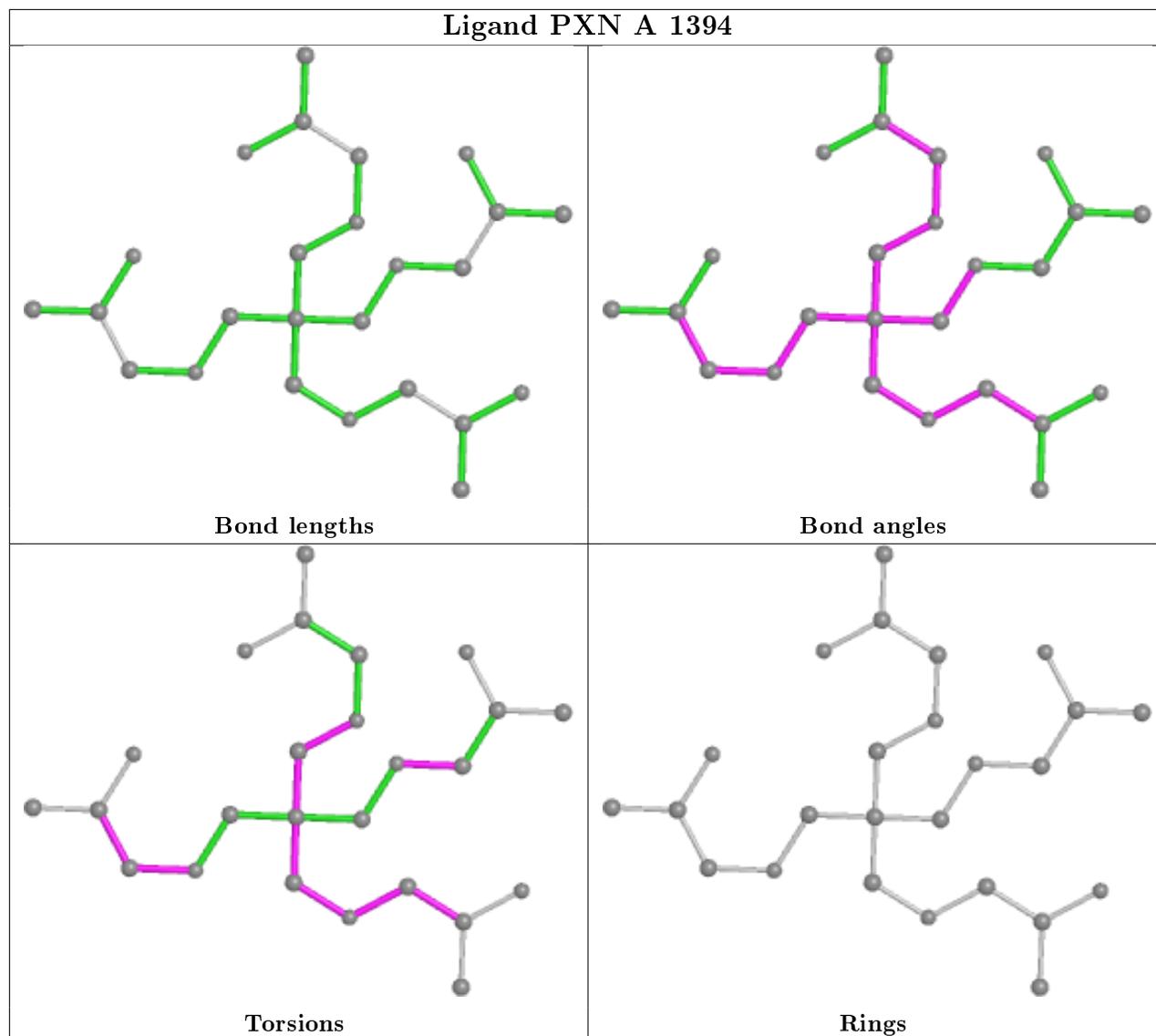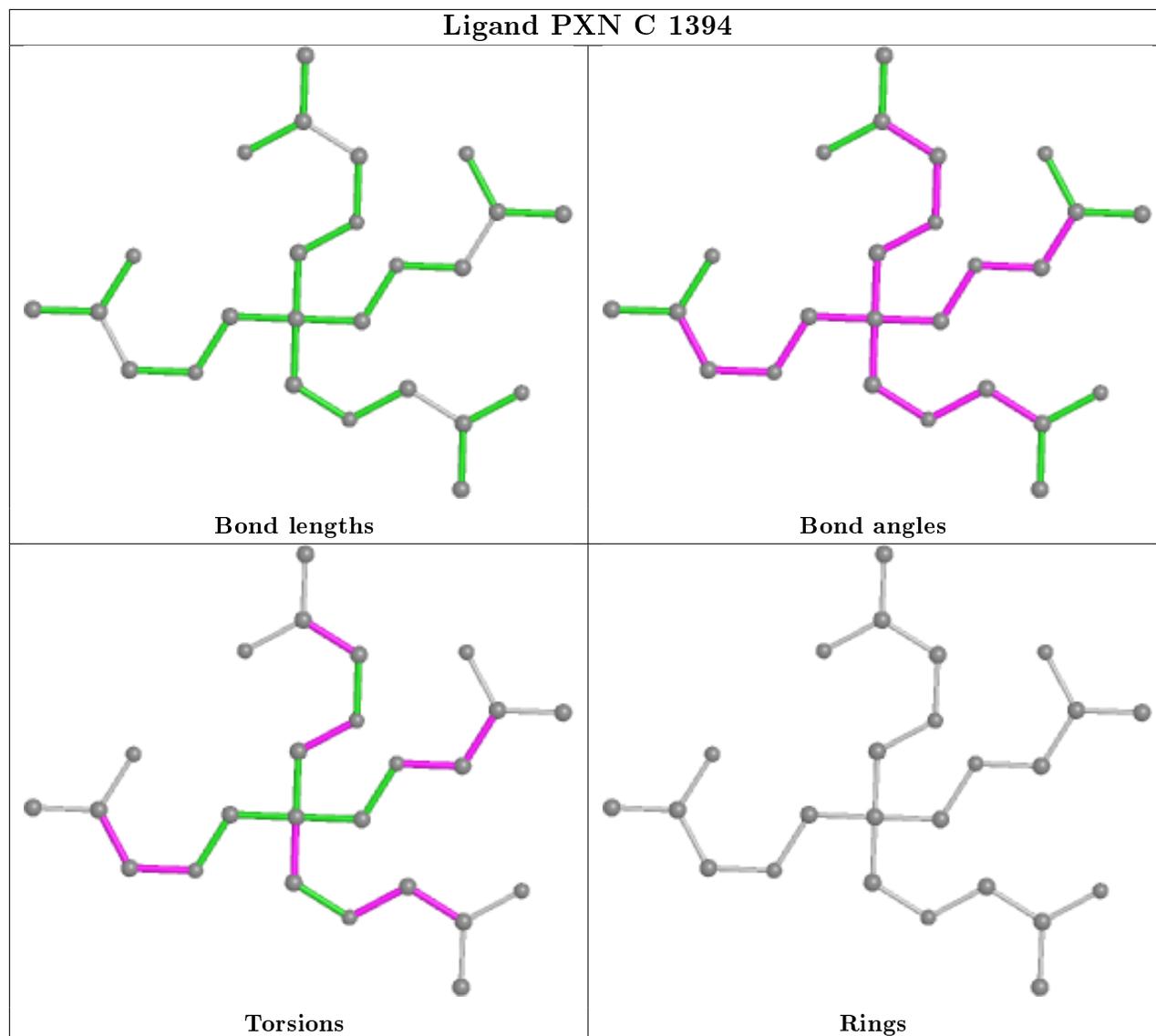
5.7 Other polymers ⓘ

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	643/678 (94%)	0.42	34 (5%)	26	28	31, 59, 109, 136	0
1	C	643/678 (94%)	0.44	46 (7%)	15	16	31, 59, 109, 136	0
2	F	549/589 (93%)	0.04	12 (2%)	62	65	23, 37, 72, 152	0
2	G	549/589 (93%)	0.21	16 (2%)	51	55	23, 37, 72, 152	0
All	All	2384/2534 (94%)	0.29	108 (4%)	33	36	23, 50, 104, 152	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	7	SER	11.6
2	F	533	CYS	9.5
2	G	533	CYS	8.2
1	C	203	GLN	7.0
1	C	1041	GLY	5.8
1	C	265	GLU	5.3
2	G	119	PHE	5.1
1	C	162	GLU	5.1
1	A	192	LYS	5.0
1	A	1064	THR	4.7
1	C	187	ALA	4.7
2	G	121	PHE	4.6
1	A	1041	GLY	4.6
2	G	519	SER	4.5
1	A	188	GLU	4.5
2	G	8	ARG	4.3
1	C	196	VAL	4.2
1	C	192	LYS	4.1
1	A	203	GLN	3.9
1	A	7	LEU	3.9
1	C	280	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	7	SER	3.8
1	C	35	LEU	3.8
1	A	199	ASP	3.8
1	C	39	ASN	3.7
1	A	198	LEU	3.7
1	C	36	ALA	3.7
1	A	187	ALA	3.7
1	C	277	ALA	3.6
2	G	535	SER	3.6
1	C	19	MET	3.5
2	G	113	PRO	3.5
2	F	119	PHE	3.5
1	A	280	LYS	3.4
2	F	121	PHE	3.4
1	C	266	LYS	3.4
1	C	1141	ASP	3.3
1	C	1324	LYS	3.3
1	A	36	ALA	3.3
1	C	28	GLU	3.2
2	F	534	ASP	3.2
1	A	281	GLN	3.1
2	G	534	ASP	3.1
1	C	15	THR	3.1
2	F	8	ARG	3.0
1	C	194	TYR	3.0
2	G	570	ARG	3.0
2	F	113	PRO	3.0
1	C	31	GLY	2.9
1	A	39	ASN	2.9
1	C	101	ALA	2.9
1	C	107	VAL	2.8
1	C	199	ASP	2.8
1	C	3	ILE	2.8
2	F	519	SER	2.8
1	A	3	ILE	2.8
2	F	537	ASP	2.8
1	C	14	ARG	2.7
1	C	195	GLN	2.7
1	A	191	GLU	2.7
1	C	198	LEU	2.7
2	G	276	SER	2.6
1	C	1393	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	47	LYS	2.6
1	A	10	GLU	2.6
1	A	157	ALA	2.5
1	A	14	ARG	2.5
1	A	162	GLU	2.5
2	F	535	SER	2.5
1	A	33	ILE	2.5
1	C	188	GLU	2.5
1	C	1064	THR	2.5
1	C	30	ASN	2.5
1	A	269	THR	2.5
1	A	1324	LYS	2.5
1	A	35	LEU	2.4
2	G	538	LEU	2.4
1	A	4	THR	2.4
1	A	1144	GLU	2.4
1	A	26	LEU	2.4
1	A	1009	LYS	2.4
1	C	33	ILE	2.4
1	C	32	ASP	2.4
1	A	140	ASP	2.3
1	A	190	VAL	2.3
1	C	1180	GLY	2.3
1	C	23	LYS	2.2
1	C	40	MET	2.2
1	C	1033	THR	2.2
1	A	24	LYS	2.2
1	C	200	ILE	2.2
1	C	281	GLN	2.2
2	G	537	ASP	2.2
1	C	267	VAL	2.2
1	A	161	ASP	2.2
2	G	112	ARG	2.2
1	A	1097	GLN	2.1
2	F	120	ASN	2.1
1	C	4	THR	2.1
2	G	571	VAL	2.1
2	G	572	LEU	2.1
1	A	32	ASP	2.1
2	F	385	LYS	2.1
1	C	116	GLU	2.1
1	C	112	ALA	2.0

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	C	1155	GLU	2.0
1	C	227	SER	2.0
1	A	265	GLU	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 carbohydrates 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($Å^2$)	Q<0.9
3	PXN	C	1394	25/25	0.85	0.25	68,73,80,80	0
3	PXN	A	1394	25/25	0.89	0.22	54,61,79,81	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 PXN C 1394:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
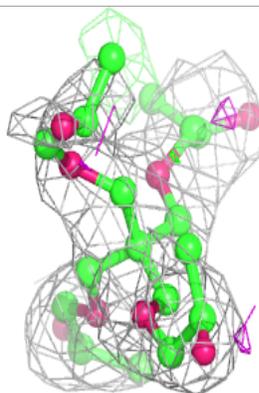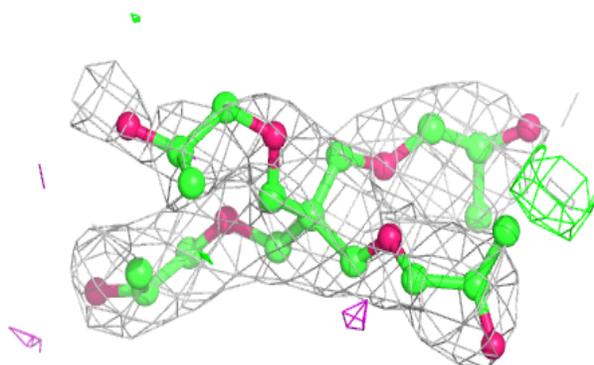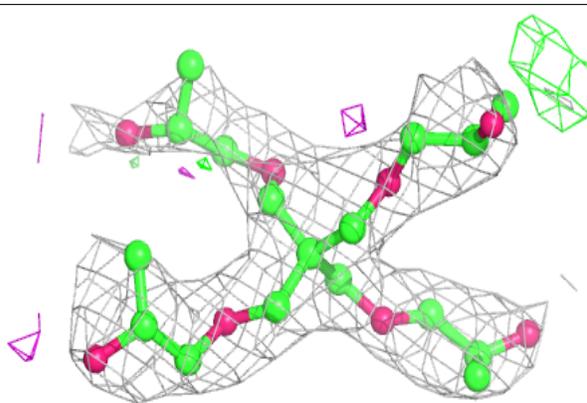
Electron density around PXN A 1394:

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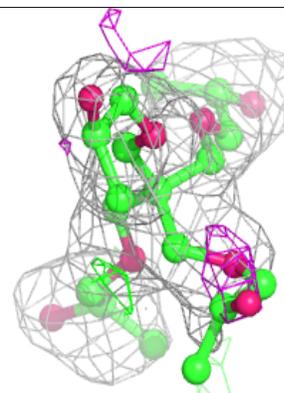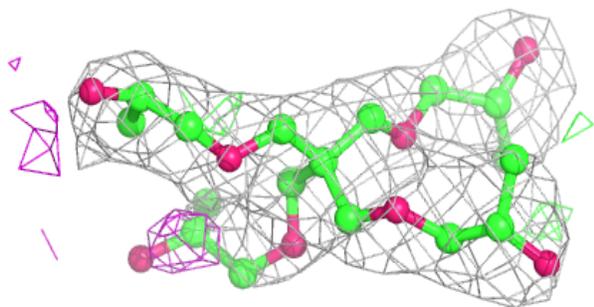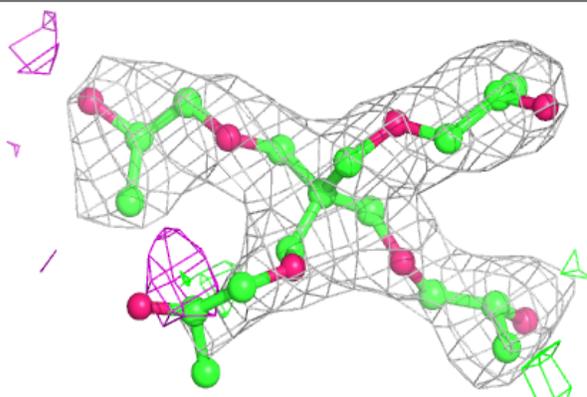
6.5 Other polymers (i)

There are no such residues in this entry.