



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:38 AM UTC

PDB ID : 2HPM / pdb_00002hpm
Title : Eubacterial and Eukaryotic Replicative DNA Polymerases are not Homologous: X-ray Structure of DNA Polymerase III
Authors : Bailey, S.; Wing, R.A.; Steitz, T.A.
Deposited on : 2006-07-17
Resolution : 3.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

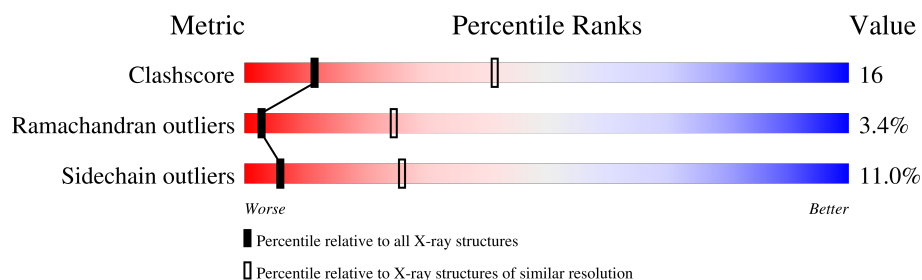
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1220	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9146 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 DNA Polymerase III alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1143	Total	C	N	O	S	0	0	0
			9127	5820	1598	1681	28			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

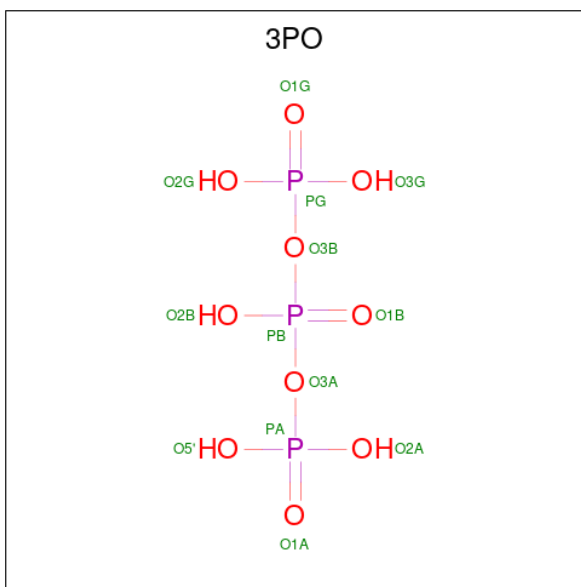
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is TRIPHOSPHATE (CCD ID: 3PO) (formula: H₅O₁₀P₃).



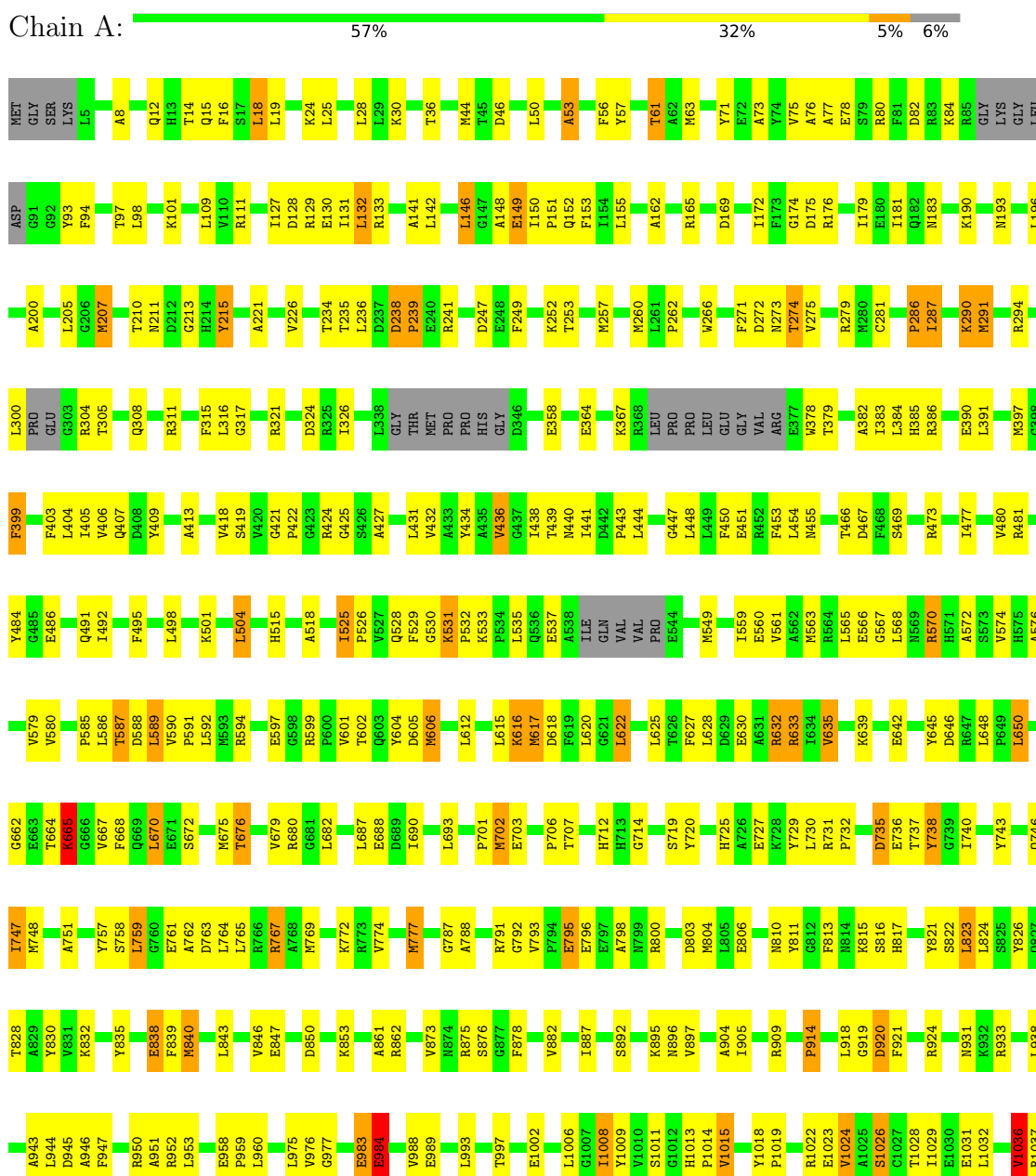
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			13	10	3		

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: DNA Polymerase III alpha subunit



F1205	LEU	GLN	GLY	ASN	GLY	GLY	GLY	GLY	PRO	LYS	GLU	GLU	VAL	VAL	PRO	PHE																																								
	E1104	V1105	E1106	LYS	GLY	GLU	GLU	LEU	R1112	A1115	V1118	W1119	T1120	A1127	F1128	K1129	A1130	L1131	V1135	K1143	G1144	VAL	A1146	R1147	G1157	S1158	L1159	L1173	F1174	A1175	L1176	R1177	E1178	V1179	R1180	V1181	G1182	E1183	E1184	A1185	L1189	E1190	A1191	E1192	G1193	Y1194	P1200	D1201	R1202	E1203	V1204					
	E1038	L1039	P1040	G1041	K1042	P1043	K1044	V1045	L1046	M1050	E1053	V1054	VAL	ARG	LYS	PRO	THR	ARG	SER	GLY	GLY	MET	MET	ALA	R1067	F1068	S1071	D1072	E1073	T1074	G1075	V1079	V1080	VAL	PHE	GLY	ARG	ALA	TYR	GLU	GLY	VAL	SER	PRO	LYS	LEU	K1094	E1095	D1096	I1097	P1098	L1099	L1100	V1101	L1102	A1103

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.44Å 185.72Å 125.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70	Depositor
% Data completeness (in resolution range)	99.9 (20.00-3.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.311	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9146	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL, MG, 3PO

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	0.64	2/9307 (0.0%)	0.98	18/12562 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	ARG	CZ-NH2	16.40	1.54	1.33
1	A	767	ARG	CZ-NH1	-13.78	1.13	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1036	VAL	N-CA-C	7.19	117.28	110.74
1	A	895	LYS	N-CA-C	6.60	119.47	111.82
1	A	438	ILE	N-CA-C	-6.37	104.94	110.74
1	A	399	PHE	CA-C-N	-6.30	111.97	119.84
1	A	399	PHE	C-N-CA	-6.30	111.97	119.84
1	A	531	LYS	CA-C-N	6.15	126.12	119.78
1	A	531	LYS	C-N-CA	6.15	126.12	119.78
1	A	378	TRP	N-CA-C	6.06	119.07	108.52
1	A	1075	GLY	N-CA-C	6.03	118.72	110.69
1	A	421	GLY	CA-C-N	5.62	126.87	119.84
1	A	421	GLY	C-N-CA	5.62	126.87	119.84
1	A	1042	LYS	CA-C-N	5.47	125.67	120.31
1	A	1042	LYS	C-N-CA	5.47	125.67	120.31
1	A	767	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	813	PHE	N-CA-C	5.35	118.00	109.81
1	A	1071	SER	N-CA-C	5.34	117.61	108.90
1	A	1127	ALA	CA-C-N	5.05	125.04	119.89
1	A	1127	ALA	C-N-CA	5.05	125.04	119.89

There are no chirality outliers.

There are no planarity outliers.

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	9127	0	9158	292	0
2	A	2	0	0	0	0
3	A	2	0	0	0	0
4	A	2	0	0	0	0
5	A	13	0	0	0	0
All	All	9146	0	9158	292	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (292) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:PRO:HB2	1:A:1050:MET:HE3	1.36	1.06
1:A:1143:LYS:HA	1:A:1147:ARG:HB2	1.43	0.96
1:A:1039:LEU:HB3	1:A:1040:PRO:CD	2.01	0.90
1:A:772:LYS:HE3	1:A:810:ASN:HD21	1.36	0.90
1:A:672:SER:HB2	1:A:675:MET:HB3	1.56	0.85
1:A:1053:GLU:HB3	1:A:1068:PHE:HA	1.58	0.84
1:A:80:ARG:N	1:A:128:ASP:OD1	2.09	0.84
1:A:703:GLU:O	1:A:706:PRO:HD2	1.78	0.83
1:A:406:VAL:HA	1:A:409:TYR:CE2	2.13	0.82
1:A:287:ILE:H	1:A:290:LYS:HG3	1.43	0.82
1:A:406:VAL:HG22	1:A:617:MET:HE1	1.59	0.81
1:A:743:TYR:H	1:A:746:GLN:HE21	1.24	0.81
1:A:257:MET:HE2	1:A:257:MET:HA	1.63	0.78
1:A:432:VAL:O	1:A:436:VAL:HG23	1.83	0.78
1:A:1013:HIS:HD2	1:A:1015:VAL:H	1.32	0.78
1:A:1039:LEU:HB3	1:A:1040:PRO:HD3	1.65	0.78
1:A:950:ARG:HA	1:A:953:LEU:HD12	1.66	0.77
1:A:951:ALA:HB2	1:A:993:LEU:HG	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:LEU:HD13	1:A:1118:VAL:HG11	1.68	0.75
1:A:111:ARG:HG2	1:A:587:THR:HG22	1.68	0.75
1:A:743:TYR:H	1:A:746:GLN:NE2	1.86	0.74
1:A:795:GLU:HA	1:A:798:ALA:HB3	1.69	0.74
1:A:238:ASP:HB3	1:A:239:PRO:O	1.89	0.72
1:A:77:ALA:O	1:A:129:ARG:NH2	2.24	0.70
1:A:850:ASP:HB3	1:A:853:LYS:HB2	1.72	0.70
1:A:1014:PRO:CB	1:A:1050:MET:HE3	2.18	0.70
1:A:958:GLU:HB3	1:A:959:PRO:HD3	1.74	0.70
1:A:169:ASP:HA	1:A:172:ILE:HD12	1.75	0.68
1:A:128:ASP:HB2	1:A:131:ILE:HG12	1.76	0.67
1:A:1026:SER:HB3	1:A:1202:ARG:HH21	1.58	0.67
1:A:701:PRO:HG3	1:A:811:TYR:HB3	1.77	0.67
1:A:97:THR:HB	1:A:142:LEU:HB2	1.78	0.66
1:A:1039:LEU:CB	1:A:1040:PRO:HD3	2.26	0.64
1:A:616:LYS:C	1:A:617:MET:HG2	2.22	0.64
1:A:1053:GLU:CB	1:A:1068:PHE:HA	2.27	0.64
1:A:311:ARG:HG2	1:A:391:LEU:HD22	1.79	0.64
1:A:920:ASP:O	1:A:924:ARG:HG3	1.98	0.64
1:A:630:GLU:OE1	1:A:633:ARG:NH1	2.31	0.64
1:A:682:LEU:HD23	1:A:693:LEU:HD22	1.81	0.63
1:A:93:TYR:O	1:A:93:TYR:CD1	2.51	0.63
1:A:635:VAL:HG23	1:A:838:GLU:HG3	1.80	0.63
1:A:179:ILE:HG23	1:A:196:LEU:HD22	1.80	0.63
1:A:419:SER:HB2	1:A:469:SER:HB2	1.82	0.62
1:A:1072:ASP:C	1:A:1074:THR:H	2.08	0.62
1:A:8:ALA:H	1:A:274:THR:HG21	1.65	0.62
1:A:148:ALA:O	1:A:152:GLN:HB2	2.00	0.62
1:A:515:HIS:O	1:A:518:ALA:HB3	1.99	0.62
1:A:840:MET:HG2	1:A:861:ALA:HB2	1.82	0.62
1:A:560:GLU:O	1:A:563:MET:HG2	2.00	0.61
1:A:239:PRO:C	1:A:241:ARG:H	2.07	0.61
1:A:98:LEU:HD11	1:A:132:LEU:HD21	1.82	0.61
1:A:1102:LEU:HD12	1:A:1119:TRP:HH2	1.66	0.61
1:A:642:GLU:OE1	1:A:642:GLU:HA	2.01	0.60
1:A:931:ASN:OD1	1:A:933:ARG:HB3	2.01	0.60
1:A:952:ARG:HG2	1:A:988:VAL:O	2.00	0.60
1:A:769:MET:HE2	1:A:806:GLU:HB3	1.83	0.60
1:A:840:MET:HB3	1:A:887:ILE:HD11	1.83	0.60
1:A:761:GLU:HA	1:A:764:LEU:HD12	1.84	0.60
1:A:94:PHE:HD2	1:A:149:GLU:HA	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1131:LEU:HD21	1:A:1189:LEU:HD23	1.84	0.59
1:A:897:VAL:HG21	1:A:938:LEU:HD13	1.84	0.59
1:A:1039:LEU:CB	1:A:1040:PRO:CD	2.77	0.59
1:A:93:TYR:O	1:A:93:TYR:HD1	1.86	0.59
1:A:1176:LEU:CD2	1:A:1179:VAL:HB	2.33	0.59
1:A:1181:VAL:HG11	1:A:1185:ALA:HB3	1.84	0.59
1:A:743:TYR:HB2	1:A:746:GLN:HG3	1.84	0.58
1:A:238:ASP:HB3	1:A:239:PRO:C	2.29	0.58
1:A:252:LYS:HD2	1:A:257:MET:HE3	1.86	0.57
1:A:1176:LEU:HD21	1:A:1179:VAL:HB	1.86	0.57
1:A:390:GLU:CD	1:A:431:LEU:H	2.11	0.57
1:A:701:PRO:O	1:A:702:MET:C	2.47	0.57
1:A:174:GLY:C	1:A:176:ARG:H	2.13	0.57
1:A:397:MET:SD	1:A:454:LEU:HD22	2.45	0.57
1:A:379:THR:HG23	1:A:382:ALA:H	1.70	0.56
1:A:427:ALA:HA	1:A:453:PHE:CD1	2.39	0.56
1:A:835:TYR:HB3	1:A:838:GLU:CG	2.35	0.56
1:A:896:ASN:ND2	1:A:933:ARG:HE	2.02	0.56
1:A:1157:GLY:N	1:A:1180:ARG:O	2.38	0.56
1:A:526:PRO:HG2	1:A:533:LYS:HD2	1.86	0.56
1:A:650:LEU:HA	1:A:826:TYR:CZ	2.41	0.56
1:A:1192:GLU:O	1:A:1194:TYR:N	2.34	0.56
1:A:1129:LYS:O	1:A:1159:LEU:HD22	2.05	0.55
1:A:1181:VAL:HG11	1:A:1185:ALA:CB	2.36	0.55
1:A:128:ASP:HB3	1:A:130:GLU:H	1.71	0.55
1:A:236:LEU:O	1:A:241:ARG:NE	2.40	0.55
1:A:150:ILE:N	1:A:151:PRO:HD2	2.21	0.55
1:A:873:VAL:HG22	1:A:943:ALA:O	2.07	0.55
1:A:1026:SER:HB3	1:A:1202:ARG:NH2	2.21	0.55
1:A:712:HIS:HD1	1:A:738:TYR:HE1	1.54	0.54
1:A:796:GLU:OE2	1:A:800:ARG:NH1	2.40	0.54
1:A:447:GLY:H	1:A:815:LYS:HZ3	1.55	0.54
1:A:16:PHE:HB2	1:A:46:ASP:OD2	2.08	0.54
1:A:1046:LEU:HA	1:A:1101:VAL:O	2.07	0.54
1:A:788:ALA:HB1	1:A:793:VAL:CG2	2.38	0.54
1:A:1143:LYS:CA	1:A:1147:ARG:HB2	2.30	0.54
1:A:183:ASN:HD22	1:A:260:MET:HB3	1.72	0.53
1:A:15:GLN:HE21	1:A:25:LEU:HB2	1.73	0.53
1:A:94:PHE:CD2	1:A:149:GLU:HA	2.44	0.53
1:A:501:LYS:HB2	1:A:532:PRO:HG3	1.91	0.53
1:A:287:ILE:N	1:A:290:LYS:HG3	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:TYR:O	1:A:746:GLN:HB2	2.09	0.52
1:A:800:ARG:HA	1:A:803:ASP:HB2	1.91	0.52
1:A:815:LYS:O	1:A:816:SER:C	2.51	0.52
1:A:720:TYR:CE1	1:A:731:ARG:HG2	2.44	0.52
1:A:846:VAL:HG12	1:A:847:GLU:HG2	1.92	0.52
1:A:315:PHE:C	1:A:317:GLY:H	2.16	0.51
1:A:586:LEU:HD13	1:A:592:LEU:HD21	1.93	0.51
1:A:93:TYR:CD1	1:A:93:TYR:C	2.89	0.51
1:A:528:GLN:HB3	1:A:533:LYS:HE3	1.93	0.51
1:A:777:MET:HA	1:A:777:MET:HE2	1.92	0.51
1:A:862:ARG:HH22	1:A:1011:SER:H	1.56	0.51
1:A:390:GLU:CD	1:A:450:PHE:CD1	2.89	0.51
1:A:467:ASP:CG	1:A:622:LEU:HD12	2.35	0.51
1:A:1192:GLU:C	1:A:1194:TYR:H	2.19	0.51
1:A:78:GLU:HB2	1:A:82:ASP:OD2	2.11	0.51
1:A:616:LYS:HG2	1:A:617:MET:N	2.25	0.51
1:A:193:ASN:HA	1:A:196:LEU:HB2	1.92	0.51
1:A:730:LEU:O	1:A:731:ARG:C	2.53	0.51
1:A:294:ARG:NH1	1:A:612:LEU:O	2.44	0.50
1:A:1040:PRO:HD2	1:A:1043:PRO:HG3	1.93	0.50
1:A:71:TYR:CD2	1:A:73:ALA:HB2	2.45	0.50
1:A:1203:GLU:O	1:A:1205:PHE:N	2.45	0.50
1:A:210:THR:O	1:A:211:ASN:HB3	2.12	0.50
1:A:662:GLY:HA3	1:A:680:ARG:HG3	1.92	0.50
1:A:1039:LEU:CG	1:A:1040:PRO:HD3	2.41	0.50
1:A:434:TYR:CD2	1:A:443:PRO:HD3	2.47	0.50
1:A:286:PRO:HA	1:A:290:LYS:HG3	1.93	0.50
1:A:413:ALA:HB1	1:A:418:VAL:HB	1.92	0.49
1:A:838:GLU:O	1:A:839:PHE:C	2.55	0.49
1:A:944:LEU:HD23	1:A:947:PHE:CE1	2.48	0.49
1:A:181:ILE:HD13	1:A:266:TRP:CZ3	2.47	0.49
1:A:57:TYR:O	1:A:61:THR:HB	2.13	0.49
1:A:80:ARG:NH1	1:A:128:ASP:OD2	2.44	0.49
1:A:618:ASP:HB3	1:A:620:LEU:HD12	1.95	0.49
1:A:153:PHE:CB	1:A:162:ALA:HB2	2.43	0.49
1:A:840:MET:SD	1:A:861:ALA:HB2	2.52	0.49
1:A:127:ILE:HD12	1:A:132:LEU:HG	1.95	0.48
1:A:480:VAL:HG13	1:A:484:TYR:HD1	1.77	0.48
1:A:720:TYR:HE1	1:A:731:ARG:HG2	1.78	0.48
1:A:840:MET:HA	1:A:843:LEU:HD12	1.94	0.48
1:A:451:GLU:OE1	1:A:451:GLU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:952:ARG:HH21	1:A:989:GLU:HG2	1.78	0.48
1:A:664:THR:O	1:A:665:LYS:C	2.56	0.48
1:A:628:LEU:HB3	1:A:645:TYR:CE1	2.49	0.48
1:A:8:ALA:H	1:A:274:THR:CG2	2.26	0.48
1:A:406:VAL:CG2	1:A:617:MET:HE1	2.38	0.47
1:A:737:THR:HG21	1:A:746:GLN:OE1	2.14	0.47
1:A:149:GLU:O	1:A:153:PHE:HD1	1.97	0.47
1:A:315:PHE:C	1:A:317:GLY:N	2.71	0.47
1:A:662:GLY:HA3	1:A:680:ARG:CG	2.45	0.47
1:A:1036:VAL:O	1:A:1037:ARG:C	2.56	0.47
1:A:14:THR:C	1:A:16:PHE:N	2.72	0.47
1:A:12:GLN:OE1	1:A:213:GLY:HA3	2.14	0.47
1:A:727:GLU:C	1:A:729:TYR:H	2.23	0.47
1:A:133:ARG:HA	1:A:172:ILE:HG23	1.97	0.47
1:A:200:ALA:HA	1:A:205:LEU:HB2	1.97	0.47
1:A:1018:TYR:CE1	1:A:1098:PRO:HG3	2.49	0.47
1:A:128:ASP:HB3	1:A:130:GLU:N	2.30	0.46
1:A:239:PRO:C	1:A:241:ARG:N	2.73	0.46
1:A:787:GLY:O	1:A:791:ARG:HG2	2.15	0.46
1:A:290:LYS:H	1:A:290:LYS:HG2	1.60	0.46
1:A:441:ILE:HD12	1:A:823:LEU:HD12	1.97	0.46
1:A:455:ASN:ND2	1:A:763:ASP:HB3	2.30	0.46
1:A:591:PRO:HD3	1:A:604:TYR:CE1	2.51	0.46
1:A:308:GLN:O	1:A:311:ARG:HB2	2.16	0.46
1:A:481:ARG:HD2	1:A:486:GLU:OE2	2.14	0.46
1:A:747:ILE:O	1:A:748:MET:C	2.59	0.46
1:A:632:ARG:O	1:A:632:ARG:HG2	2.13	0.46
1:A:1099:LEU:HD13	1:A:1118:VAL:CG1	2.43	0.46
1:A:274:THR:CG2	1:A:275:VAL:N	2.78	0.46
1:A:473:ARG:NH1	1:A:576:ALA:O	2.49	0.46
1:A:667:VAL:HA	1:A:828:THR:HG21	1.97	0.46
1:A:840:MET:CG	1:A:861:ALA:HB2	2.46	0.46
1:A:1072:ASP:C	1:A:1074:THR:N	2.72	0.46
1:A:179:ILE:HG13	1:A:200:ALA:HB2	1.98	0.46
1:A:525:ILE:HA	1:A:526:PRO:HD3	1.84	0.46
1:A:1006:LEU:C	1:A:1008:ILE:H	2.24	0.46
1:A:529:PHE:O	1:A:531:LYS:N	2.45	0.45
1:A:153:PHE:HB2	1:A:162:ALA:HB2	1.97	0.45
1:A:712:HIS:C	1:A:714:GLY:H	2.23	0.45
1:A:1008:ILE:HD12	1:A:1009:TYR:O	2.16	0.45
1:A:364:GLU:HA	1:A:367:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:HIS:CD2	1:A:1015:VAL:H	2.23	0.45
1:A:591:PRO:C	1:A:592:LEU:HG	2.42	0.45
1:A:141:ALA:O	1:A:142:LEU:HD23	2.17	0.45
1:A:585:PRO:O	1:A:588:ASP:HB2	2.16	0.45
1:A:1159:LEU:HD11	1:A:1183:GLU:HG2	1.99	0.45
1:A:76:ALA:O	1:A:77:ALA:C	2.60	0.45
1:A:215:TYR:CE1	1:A:249:PHE:HB2	2.52	0.45
1:A:747:ILE:HG22	1:A:748:MET:N	2.31	0.45
1:A:648:LEU:HD22	1:A:830:TYR:CE2	2.51	0.44
1:A:1044:LYS:HA	1:A:1104:GLU:HA	1.98	0.44
1:A:405:ILE:O	1:A:409:TYR:HD2	2.00	0.44
1:A:574:VAL:HG21	1:A:599:ARG:HD2	1.99	0.44
1:A:840:MET:O	1:A:843:LEU:HB2	2.17	0.44
1:A:918:LEU:HD22	1:A:953:LEU:HD23	1.99	0.44
1:A:1105:VAL:HG12	1:A:1106:GLU:N	2.32	0.44
1:A:422:PRO:HA	1:A:440:ASN:HB3	2.00	0.44
1:A:425:GLY:HA2	1:A:817:HIS:HB2	2.00	0.44
1:A:238:ASP:HB3	1:A:239:PRO:CA	2.47	0.44
1:A:405:ILE:O	1:A:409:TYR:CD2	2.71	0.44
1:A:840:MET:HA	1:A:840:MET:HE2	2.00	0.44
1:A:795:GLU:HA	1:A:798:ALA:CB	2.45	0.44
1:A:1029:ILE:HG12	1:A:1072:ASP:CG	2.42	0.44
1:A:24:LYS:HE2	1:A:567:GLY:H	1.82	0.44
1:A:305:THR:HB	1:A:308:GLN:H	1.82	0.44
1:A:840:MET:HE3	1:A:840:MET:HB2	1.76	0.44
1:A:1181:VAL:CG1	1:A:1182:GLY:N	2.81	0.44
1:A:664:THR:HG1	1:A:676:THR:HG1	1.64	0.44
1:A:617:MET:HE2	1:A:617:MET:HB3	1.73	0.44
1:A:693:LEU:HD12	1:A:693:LEU:HA	1.77	0.44
1:A:492:ILE:HA	1:A:602:THR:HB	2.00	0.43
1:A:758:SER:O	1:A:761:GLU:N	2.51	0.43
1:A:447:GLY:N	1:A:815:LYS:HZ3	2.16	0.43
1:A:878:PHE:CE1	1:A:892:SER:HB3	2.53	0.43
1:A:215:TYR:CD1	1:A:215:TYR:N	2.86	0.43
1:A:279:ARG:C	1:A:281:CYS:H	2.26	0.43
1:A:399:PHE:O	1:A:403:PHE:HD1	2.01	0.43
1:A:751:ALA:HB1	1:A:757:TYR:HD1	1.82	0.43
1:A:1039:LEU:HB3	1:A:1040:PRO:HD2	1.95	0.43
1:A:862:ARG:NH2	1:A:1011:SER:H	2.16	0.43
1:A:1028:THR:HG23	1:A:1031:GLU:H	1.84	0.43
1:A:211:ASN:O	1:A:211:ASN:CG	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD12	1:A:525:ILE:HD11	2.00	0.43
1:A:701:PRO:HD3	1:A:811:TYR:CD2	2.53	0.43
1:A:821:TYR:O	1:A:822:SER:C	2.62	0.43
1:A:385:HIS:O	1:A:386:ARG:C	2.62	0.43
1:A:735:ASP:C	1:A:737:THR:H	2.27	0.43
1:A:821:TYR:O	1:A:824:LEU:N	2.49	0.43
1:A:835:TYR:HB3	1:A:838:GLU:HG2	2.01	0.43
1:A:14:THR:C	1:A:16:PHE:H	2.25	0.43
1:A:93:TYR:HD1	1:A:93:TYR:C	2.27	0.43
1:A:257:MET:HA	1:A:257:MET:CE	2.40	0.43
1:A:379:THR:O	1:A:383:ILE:HG13	2.18	0.43
1:A:424:ARG:HB3	1:A:821:TYR:HE1	1.84	0.43
1:A:525:ILE:H	1:A:525:ILE:HG13	1.39	0.43
1:A:731:ARG:O	1:A:732:PRO:C	2.62	0.43
1:A:1024:VAL:HG21	1:A:1200:PRO:HB2	2.00	0.43
1:A:675:MET:O	1:A:679:VAL:HG23	2.17	0.43
1:A:570:ARG:HD3	1:A:570:ARG:HA	1.77	0.43
1:A:1176:LEU:HD23	1:A:1179:VAL:HB	2.01	0.43
1:A:491:GLN:O	1:A:601:VAL:HA	2.18	0.42
1:A:391:LEU:HG	1:A:432:VAL:HG21	2.00	0.42
1:A:838:GLU:HA	1:A:882:VAL:HG21	2.01	0.42
1:A:919:GLY:C	1:A:921:PHE:N	2.78	0.42
1:A:1028:THR:HG22	1:A:1031:GLU:OE1	2.20	0.42
1:A:1143:LYS:C	1:A:1147:ARG:H	2.28	0.42
1:A:207:MET:HE2	1:A:207:MET:HB2	1.96	0.42
1:A:586:LEU:C	1:A:588:ASP:N	2.77	0.42
1:A:670:LEU:HA	1:A:675:MET:HG2	2.00	0.42
1:A:727:GLU:C	1:A:729:TYR:N	2.78	0.42
1:A:1103:ALA:CB	1:A:1115:ALA:HA	2.50	0.42
1:A:174:GLY:O	1:A:176:ARG:N	2.50	0.42
1:A:904:ALA:O	1:A:905:ILE:C	2.62	0.42
1:A:1018:TYR:HA	1:A:1019:PRO:HD3	1.81	0.42
1:A:127:ILE:CD1	1:A:132:LEU:HG	2.50	0.42
1:A:832:LYS:HB2	1:A:839:PHE:CE1	2.54	0.42
1:A:226:VAL:HG21	1:A:561:VAL:HG11	2.01	0.42
1:A:687:LEU:O	1:A:690:ILE:N	2.53	0.42
1:A:909:ARG:O	1:A:909:ARG:HG2	2.20	0.42
1:A:1002:GLU:O	1:A:1006:LEU:N	2.53	0.42
1:A:983:GLU:O	1:A:984:GLU:C	2.63	0.41
1:A:1201:ASP:OD1	1:A:1201:ASP:C	2.61	0.41
1:A:44:MET:SD	1:A:53:ALA:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:VAL:HA	1:A:591:PRO:HD3	1.94	0.41
1:A:701:PRO:O	1:A:703:GLU:N	2.53	0.41
1:A:1067:ARG:HA	1:A:1080:VAL:HG22	2.02	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.83	0.41
1:A:495:PHE:HE2	1:A:572:ALA:HB2	1.85	0.41
1:A:682:LEU:HD22	1:A:693:LEU:HD13	2.02	0.41
1:A:765:LEU:O	1:A:769:MET:HG3	2.20	0.41
1:A:737:THR:HG23	1:A:740:ILE:H	1.85	0.41
1:A:759:LEU:O	1:A:762:ALA:HB3	2.21	0.41
1:A:945:ASP:C	1:A:947:PHE:H	2.28	0.41
1:A:44:MET:HB2	1:A:56:PHE:CE2	2.55	0.41
1:A:290:LYS:HB2	1:A:291:MET:H	1.73	0.41
1:A:712:HIS:C	1:A:714:GLY:N	2.78	0.41
1:A:404:LEU:O	1:A:405:ILE:C	2.64	0.41
1:A:1175:ALA:O	1:A:1176:LEU:O	2.39	0.41
1:A:271:PHE:C	1:A:273:ASN:H	2.29	0.41
1:A:594:ARG:HA	1:A:599:ARG:O	2.20	0.41
1:A:1189:LEU:C	1:A:1191:ALA:N	2.78	0.41
1:A:97:THR:HG21	1:A:142:LEU:HD12	2.03	0.40
1:A:434:TYR:CD2	1:A:443:PRO:CD	3.04	0.40
1:A:605:ASP:O	1:A:606:MET:C	2.65	0.40
1:A:665:LYS:H	1:A:665:LYS:HG3	1.71	0.40
1:A:725:HIS:HB2	1:A:793:VAL:HG12	2.03	0.40
1:A:448:LEU:HD22	1:A:816:SER:HA	2.02	0.40
1:A:627:PHE:HA	1:A:846:VAL:HG21	2.04	0.40
1:A:549:MET:HG3	1:A:559:ILE:CD1	2.50	0.40
1:A:838:GLU:CD	1:A:838:GLU:H	2.29	0.40
1:A:565:LEU:O	1:A:566:GLU:C	2.63	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	1123/1220 (92%)	939 (84%)	146 (13%)	38 (3%)	3	25

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	ALA
1	A	175	ASP
1	A	221	ALA
1	A	702	MET
1	A	774	VAL
1	A	1039	LEU
1	A	1176	LEU
1	A	1204	VAL
1	A	18	LEU
1	A	146	LEU
1	A	530	GLY
1	A	587	THR
1	A	665	LYS
1	A	975	LEU
1	A	983	GLU
1	A	1040	PRO
1	A	1177	ARG
1	A	1193	GLY
1	A	262	PRO
1	A	272	ASP
1	A	589	LEU
1	A	606	MET
1	A	738	TYR
1	A	914	PRO
1	A	920	ASP
1	A	286	PRO
1	A	291	MET
1	A	570	ARG
1	A	946	ALA
1	A	984	GLU
1	A	668	PHE
1	A	976	VAL
1	A	977	GLY
1	A	688	GLU
1	A	1203	GLU
1	A	792	GLY
1	A	238	ASP
1	A	239	PRO

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	949/1009 (94%)	845 (89%)	104 (11%)	6 26

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	19	LEU
1	A	28	LEU
1	A	30	LYS
1	A	36	THR
1	A	50	LEU
1	A	61	THR
1	A	63	MET
1	A	75	VAL
1	A	84	LYS
1	A	101	LYS
1	A	109	LEU
1	A	132	LEU
1	A	146	LEU
1	A	149	GLU
1	A	155	LEU
1	A	165	ARG
1	A	190	LYS
1	A	207	MET
1	A	215	TYR
1	A	234	THR
1	A	235	THR
1	A	247	ASP
1	A	253	THR
1	A	274	THR
1	A	287	ILE
1	A	290	LYS
1	A	300	LEU
1	A	304	ARG
1	A	316	LEU

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Mol	Chain	Res	Type
1	A	321	ARG
1	A	324	ASP
1	A	326	ILE
1	A	358	GLU
1	A	407	GLN
1	A	436	VAL
1	A	439	THR
1	A	444	LEU
1	A	466	THR
1	A	477	ILE
1	A	498	LEU
1	A	504	LEU
1	A	525	ILE
1	A	535	LEU
1	A	537	GLU
1	A	568	LEU
1	A	579	VAL
1	A	580	VAL
1	A	589	LEU
1	A	597	GLU
1	A	615	LEU
1	A	616	LYS
1	A	617	MET
1	A	622	LEU
1	A	625	LEU
1	A	632	ARG
1	A	633	ARG
1	A	635	VAL
1	A	639	LYS
1	A	646	ASP
1	A	650	LEU
1	A	665	LYS
1	A	670	LEU
1	A	676	THR
1	A	707	THR
1	A	719	SER
1	A	735	ASP
1	A	736	GLU
1	A	747	ILE
1	A	759	LEU
1	A	767	ARG
1	A	777	MET

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Mol	Chain	Res	Type
1	A	795	GLU
1	A	804	MET
1	A	823	LEU
1	A	838	GLU
1	A	840	MET
1	A	875	ARG
1	A	876	SER
1	A	914	PRO
1	A	960	LEU
1	A	984	GLU
1	A	997	THR
1	A	1008	ILE
1	A	1015	VAL
1	A	1022	ARG
1	A	1023	GLU
1	A	1024	VAL
1	A	1026	SER
1	A	1032	LEU
1	A	1036	VAL
1	A	1045	VAL
1	A	1074	THR
1	A	1079	VAL
1	A	1080	VAL
1	A	1095	GLU
1	A	1096	ASP
1	A	1118	VAL
1	A	1120	THR
1	A	1135	VAL
1	A	1158	SER
1	A	1173	LEU
1	A	1184	GLU
1	A	1192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	15	GLN
1	A	135	HIS
1	A	167	ASN
1	A	182	GLN
1	A	183	ASN

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Mol	Chain	Res	Type
1	A	273	ASN
1	A	440	ASN
1	A	725	HIS
1	A	746	GLN
1	A	753	GLN
1	A	810	ASN
1	A	814	ASN
1	A	827	GLN
1	A	1013	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
5	3PO	A	1227	-	10,12,12	1.55	3 (30%)	17,20,20	1.08	0

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
5	3PO	A	1227	-	-	2/12/12/12	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1227	3PO	PB-O3B	3.35	1.63	1.59
5	A	1227	3PO	PA-O1A	2.15	1.57	1.50
5	A	1227	3PO	PB-O3A	2.15	1.61	1.59

There are no bond angle outliers.

There are no chirality outliers.

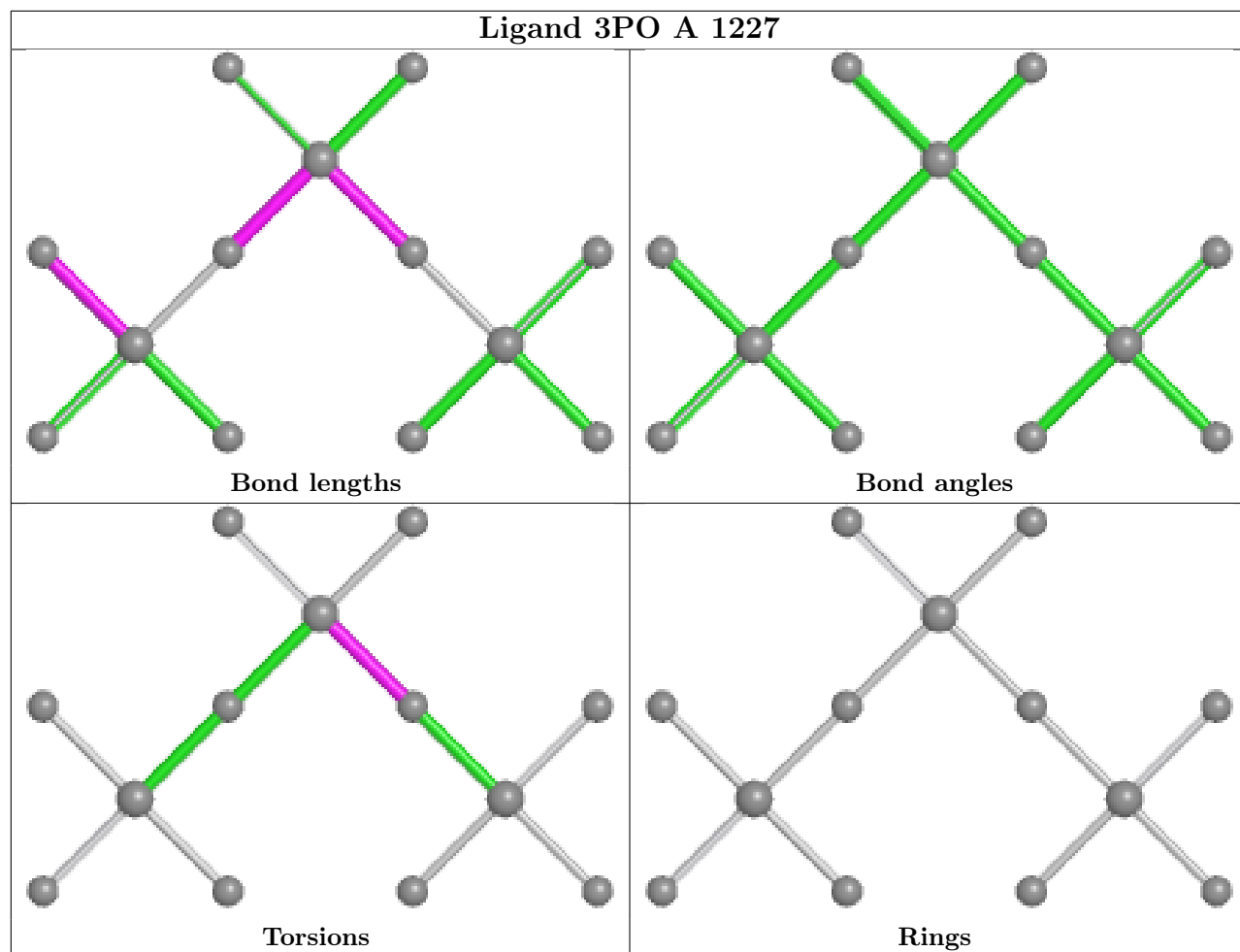
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1227	3PO	PG-O3B-PB-O2B
5	A	1227	3PO	PG-O3B-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.