



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 02:48 pm BST

PDB ID : 2HPM
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 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

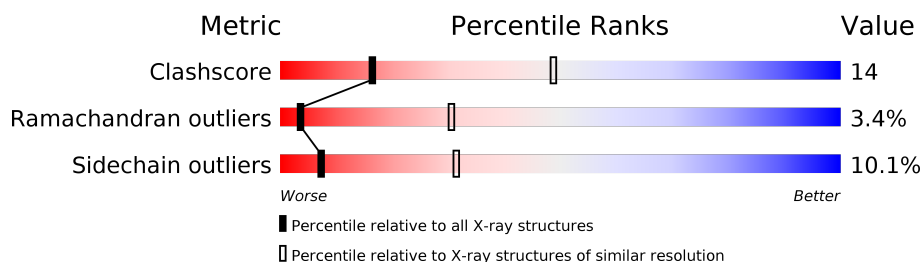
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)

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 $\leq 5\%$.

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 (three-letter code: ZN) (formula: Zn).

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

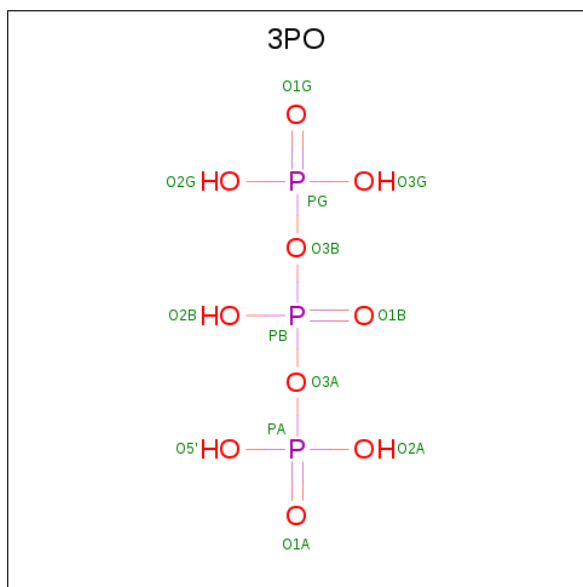
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is TRIPHOSPHATE (three-letter code: 3PO) (formula: H₅O₁₀P₃).



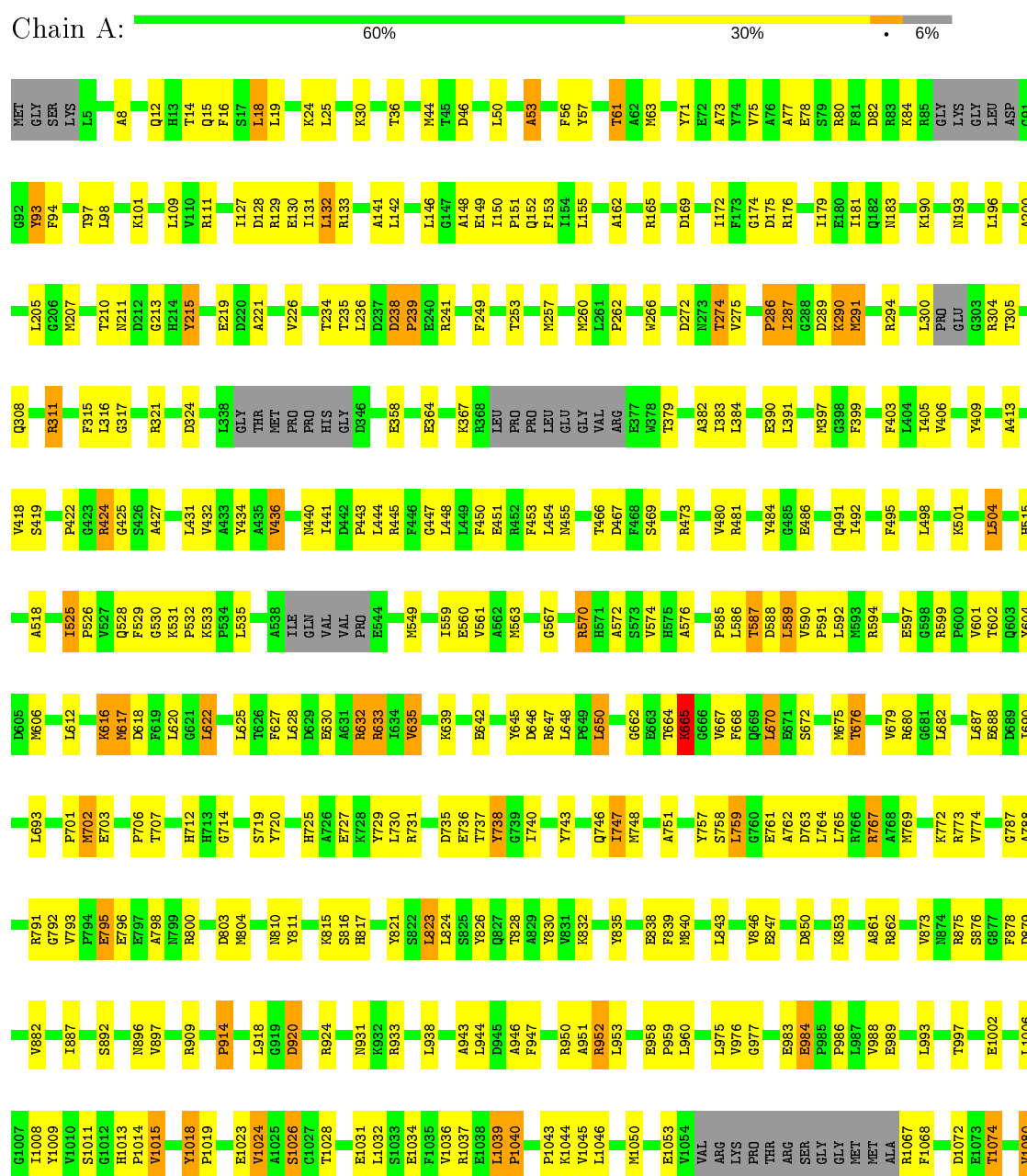
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			13	10	3		

3 Residue-property plots

These plots are drawn for all protein, RNA 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. 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



VAL	VAL
PHE	PHE
GLY	GLY
ARG	ARG
ALA	ALA
TVR	TVR
GLU	GLU
GLY	GLY
VAL	VAL
SER	SER
PRO	PRO
LYS	LYS
LEU	LEU
K1094	K1094
E1095	E1095
D1096	D1096
I1097	I1097
P1098	P1098
L1099	L1099
L1100	L1100
V1101	V1101
L1102	L1102
A1103	A1103
E1104	E1104
V1105	V1105
E1106	E1106
LYS	LYS
GLY	GLY
GLU	GLU
GLY	GLY
LEU	LEU
R1112	R1112
A1115	A1115
V1118	V1118
W1119	W1119
T1120	T1120
K1129	K1129
A1130	A1130
L1131	L1131
V1135	V1135
D1136	D1136
K1143	K1143
G1144	G1144
VAL	VAL
A1146	A1146
R1147	R1147
G1157	G1157
S1158	S1158
L1159	L1159
F1169	F1169
L1173	L1173
F1174	F1174

A1175	A1175
L1176	L1176
R1177	R1177
E1178	E1178
V1179	V1179
R1180	R1180
V1181	V1181
G1182	G1182
E1183	E1183
E1184	E1184
A1185	A1185
L1189	L1189
E1192	E1192
G1193	G1193
Y1194	Y1194
P1200	P1200
D1201	D1201
R1202	R1202
E1203	E1203
V1204	V1204
F1205	F1205
LEU	LEU
GLN	GLN
GLY	GLY
ASN	ASN
GLY	GLY
GLY	GLY
GLY	GLY
PRO	PRO
LYS	LYS
GLU	GLU
GLU	GLU
VAL	VAL
VAL	VAL
PRO	PRO
PHE	PHE

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	0.55	5/9307 (0.1%)	0.69	3/12562 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	767	ARG	CZ-NH2	16.71	1.54	1.33
1	A	767	ARG	CZ-NH1	-15.07	1.13	1.33
1	A	1034	GLU	CD-OE1	6.77	1.33	1.25
1	A	219	GLU	CD-OE2	5.80	1.32	1.25
1	A	219	GLU	CD-OE1	5.77	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	767	ARG	NE-CZ-NH1	13.13	126.86	120.30
1	A	767	ARG	NE-CZ-NH2	-10.99	114.80	120.30
1	A	1159	LEU	CA-CB-CG	5.12	127.08	115.30

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	261	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	261	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 14.

All (261) 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: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:743:TYR:H	1:A:746:GLN:HE21	1.24	0.81
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
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: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:406:VAL:HG22	1:A:617:MET:HE1	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:LEU:CB	1:A:1040:PRO:HD3	2.26	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: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:1014:PRO:HB2	1:A:1050:MET:CE	2.30	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: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:1014:PRO:HB2	1:A:1050:MET:HE2	1.83	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: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
1:A:1131:LEU:HD21	1:A:1189:LEU:HD23	1.84	0.59
1:A:1039:LEU:CB	1:A:1040:PRO:CD	2.77	0.59
1:A:897:VAL:HG21	1:A:938:LEU:HD13	1.84	0.59
1:A:616:LYS:C	1:A:617:MET:HG2	2.22	0.59
1:A:1176:LEU:CD2	1:A:1179:VAL:HB	2.33	0.59
1:A:93:TYR:O	1:A:93:TYR:HD1	1.86	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:1072:ASP:C	1:A:1074:THR:H	2.08	0.57
1:A:1176:LEU:HD21	1:A:1179:VAL:HB	1.86	0.57
1:A:239:PRO:C	1:A:241:ARG:H	2.07	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:1157:GLY:N	1:A:1180:ARG:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ASN:ND2	1:A:933:ARG:HE	2.02	0.56
1:A:526:PRO:HG2	1:A:533:LYS:HD2	1.86	0.56
1:A:1192:GLU:O	1:A:1194:TYR:N	2.34	0.56
1:A:650:LEU:HA	1:A:826:TYR:CZ	2.41	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: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:1143:LYS:CA	1:A:1147:ARG:HB2	2.30	0.54
1:A:788:ALA:HB1	1:A:793:VAL:CG2	2.38	0.54
1:A:183:ASN:HD22	1:A:260:MET:HB3	1.72	0.53
1:A:238:ASP:HB3	1:A:239:PRO:C	2.29	0.53
1:A:15:GLN:HE21	1:A:25:LEU:HB2	1.73	0.53
1:A:390:GLU:CD	1:A:431:LEU:H	2.11	0.53
1:A:501:LYS:HB2	1:A:532:PRO:HG3	1.91	0.53
1:A:701:PRO:O	1:A:702:MET:C	2.47	0.53
1:A:94:PHE:CD2	1:A:149:GLU:HA	2.44	0.53
1:A:287:ILE:N	1:A:290:LYS:HG3	2.20	0.53
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:174:GLY:C	1:A:176:ARG:H	2.13	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:616:LYS:HG2	1:A:617:MET:N	2.25	0.52
1:A:840:MET:CA	1:A:840:MET:HE2	2.40	0.51
1:A:586:LEU:HD13	1:A:592:LEU:HD21	1.93	0.51
1:A:528:GLN:HB3	1:A:533:LYS:HE3	1.93	0.51
1:A:862:ARG:HH22	1:A:1011:SER:H	1.56	0.51
1:A:257:MET:CE	1:A:257:MET:HA	2.40	0.51
1:A:78:GLU:HB2	1:A:82:ASP:OD2	2.11	0.51
1:A:193:ASN:HA	1:A:196:LEU:HB2	1.92	0.51
1:A:1040:PRO:HD2	1:A:1043:PRO:HG3	1.93	0.50
1:A:294:ARG:NH1	1:A:612:LEU:O	2.44	0.50
1:A:1203:GLU:O	1:A:1205:PHE:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:CD2	1:A:73:ALA:HB2	2.45	0.50
1:A:1039:LEU:CG	1:A:1040:PRO:HD3	2.41	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: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:840:MET:HA	1:A:840:MET:HE2	1.93	0.49
1:A:413:ALA:HB1	1:A:418:VAL:HB	1.92	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:80:ARG:NH1	1:A:128:ASP:OD2	2.44	0.49
1:A:57:TYR:O	1:A:61:THR:HB	2.13	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
1:A:952:ARG:HH21	1:A:989:GLU:HG2	1.78	0.48
1:A:628:LEU:HB3	1:A:645:TYR:CE1	2.49	0.48
1:A:815:LYS:O	1:A:816:SER:C	2.51	0.48
1:A:8:ALA:H	1:A:274:THR:CG2	2.26	0.48
1:A:632:ARG:HG2	1:A:632:ARG:O	2.13	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:H	2.16	0.47
1:A:662:GLY:HA3	1:A:680:ARG:CG	2.45	0.47
1:A:12:GLN:OE1	1:A:213:GLY:HA3	2.14	0.47
1:A:1018:TYR:CE1	1:A:1098:PRO:HG3	2.49	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:128:ASP:HB3	1:A:130:GLU:N	2.30	0.46
1:A:787:GLY:O	1:A:791:ARG:HG2	2.15	0.46
1:A:290:LYS:HG2	1:A:290:LYS:H	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:467:ASP:CG	1:A:622:LEU:HD12	2.35	0.46
1:A:591:PRO:HD3	1:A:604:TYR:CE1	2.51	0.46
1:A:93:TYR:C	1:A:93:TYR:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:O	1:A:311:ARG:HB2	2.16	0.46
1:A:390:GLU:CD	1:A:450:PHE:CD1	2.89	0.46
1:A:481:ARG:HD2	1:A:486:GLU:OE2	2.14	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:730:LEU:O	1:A:731:ARG:C	2.53	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: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:529:PHE:O	1:A:531:LYS:N	2.45	0.45
1:A:1008:ILE:HD12	1:A:1009:TYR:O	2.16	0.45
1:A:153:PHE:HB2	1:A:162:ALA:HB2	1.97	0.45
1:A:364:GLU:HA	1:A:367:LYS:HE2	1.98	0.45
1:A:1013:HIS:CD2	1:A:1015:VAL:H	2.23	0.45
1:A:1014:PRO:HB2	1:A:1050:MET:HE3	1.99	0.45
1:A:141:ALA:O	1:A:142:LEU:HD23	2.17	0.45
1:A:1159:LEU:HD11	1:A:1183:GLU:HG2	1.99	0.45
1:A:585:PRO:O	1:A:588:ASP:HB2	2.16	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:838:GLU:O	1:A:839:PHE:C	2.55	0.45
1:A:1044:LYS:HA	1:A:1104:GLU:HA	1.98	0.44
1:A:648:LEU:HD22	1:A:830:TYR:CE2	2.51	0.44
1:A:1105:VAL:HG12	1:A:1106:GLU:N	2.32	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: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:795:GLU:HA	1:A:798:ALA:CB	2.45	0.44
1:A:1181:VAL:CG1	1:A:1182:GLY:N	2.81	0.44
1:A:305:THR:HB	1:A:308:GLN:H	1.82	0.44
1:A:24:LYS:HE2	1:A:567:GLY:H	1.82	0.44
1:A:664:THR:HG1	1:A:676:THR:HG1	1.64	0.44
1:A:693:LEU:HD12	1:A:693:LEU:HA	1.77	0.44
1:A:315:PHE:C	1:A:317:GLY:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:878:PHE:CE1	1:A:892:SER:HB3	2.53	0.43
1:A:1039:LEU:HB3	1:A:1040:PRO:HD2	1.95	0.43
1:A:215:TYR:CD1	1:A:215:TYR:N	2.86	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: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:664:THR:O	1:A:665:LYS:C	2.56	0.43
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:824:LEU:N	2.49	0.43
1:A:835:TYR:HB3	1:A:838:GLU:HG2	2.01	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:1024:VAL:HG21	1:A:1200:PRO:HB2	2.00	0.43
1:A:525:ILE:HG13	1:A:525:ILE:H	1.39	0.43
1:A:675:MET:O	1:A:679:VAL:HG23	2.17	0.43
1:A:1176:LEU:HD23	1:A:1179:VAL:HB	2.01	0.43
1:A:239:PRO:C	1:A:241:ARG:N	2.73	0.43
1:A:570:ARG:HA	1:A:570:ARG:HD3	1.77	0.43
1:A:491:GLN:O	1:A:601:VAL:HA	2.18	0.42
1:A:1028:THR:HG22	1:A:1031:GLU:OE1	2.20	0.42
1:A:1036:VAL:O	1:A:1037:ARG:C	2.56	0.42
1:A:1072:ASP:C	1:A:1074:THR:N	2.72	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:727:GLU:C	1:A:729:TYR:H	2.23	0.42
1:A:406:VAL:CG2	1:A:617:MET:HE1	2.47	0.42
1:A:1103:ALA:CB	1:A:1115:ALA:HA	2.50	0.42
1:A:670:LEU:HA	1:A:675:MET:HG2	2.00	0.42
1:A:1018:TYR:HA	1:A:1019:PRO:HD3	1.81	0.42
1:A:174:GLY:O	1:A:176:ARG:N	2.50	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:1002:GLU:O	1:A:1006:LEU:N	2.53	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:14:THR:C	1:A:16:PHE:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:HIS:C	1:A:714:GLY:H	2.23	0.41
1:A:44:MET:SD	1:A:53:ALA:N	2.93	0.41
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:747:ILE:O	1:A:748:MET:C	2.59	0.41
1:A:1067:ARG:HA	1:A:1080:VAL:HG22	2.02	0.41
1:A:1192:GLU:C	1:A:1194:TYR:H	2.19	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:1006:LEU:C	1:A:1008:ILE:H	2.24	0.41
1:A:290:LYS:HB2	1:A:291:MET:H	1.73	0.41
1:A:44:MET:HB2	1:A:56:PHE:CE2	2.55	0.41
1:A:1175:ALA:O	1:A:1176:LEU:O	2.39	0.41
1:A:594:ARG:HA	1:A:599:ARG:O	2.20	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:665:LYS:HG3	1:A:665:LYS:H	1.71	0.40
1:A:725:HIS:HB2	1:A:793:VAL:HG12	2.03	0.40
1:A:447:GLY:H	1:A:815:LYS:HZ1	1.69	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:591:PRO:C	1:A:592:LEU:HG	2.42	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	30

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%)	853 (90%)	96 (10%)	7 31

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	19	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	93	TYR
1	A	101	LYS
1	A	109	LEU
1	A	132	LEU
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	253	THR
1	A	274	THR
1	A	287	ILE
1	A	289	ASP
1	A	290	LYS
1	A	300	LEU
1	A	304	ARG
1	A	311	ARG
1	A	316	LEU
1	A	321	ARG

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Mol	Chain	Res	Type
1	A	324	ASP
1	A	358	GLU
1	A	424	ARG
1	A	436	VAL
1	A	444	LEU
1	A	445	ARG
1	A	466	THR
1	A	498	LEU
1	A	504	LEU
1	A	525	ILE
1	A	535	LEU
1	A	589	LEU
1	A	597	GLU
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	647	ARG
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	773	ARG
1	A	795	GLU
1	A	804	MET
1	A	823	LEU
1	A	875	ARG
1	A	876	SER
1	A	879	ASP
1	A	914	PRO

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Mol	Chain	Res	Type
1	A	952	ARG
1	A	960	LEU
1	A	984	GLU
1	A	986	PRO
1	A	997	THR
1	A	1015	VAL
1	A	1018	TYR
1	A	1023	GLU
1	A	1024	VAL
1	A	1026	SER
1	A	1032	LEU
1	A	1045	VAL
1	A	1074	THR
1	A	1080	VAL
1	A	1095	GLU
1	A	1096	ASP
1	A	1120	THR
1	A	1135	VAL
1	A	1136	ASP
1	A	1158	SER
1	A	1169	PHE
1	A	1173	LEU
1	A	1184	GLU
1	A	1192	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	182	GLN
1	A	183	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	896	ASN
1	A	1013	HIS
1	A	1155	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	8,12,12	0.97	1 (12%)	15,20,20	1.48	2 (13%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1227	3PO	PA-O1A	2.05	1.57	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1227	3PO	PB-O3A-PA	-2.95	122.72	132.83
5	A	1227	3PO	PB-O3B-PG	-2.83	123.10	132.83

There are no chirality outliers.

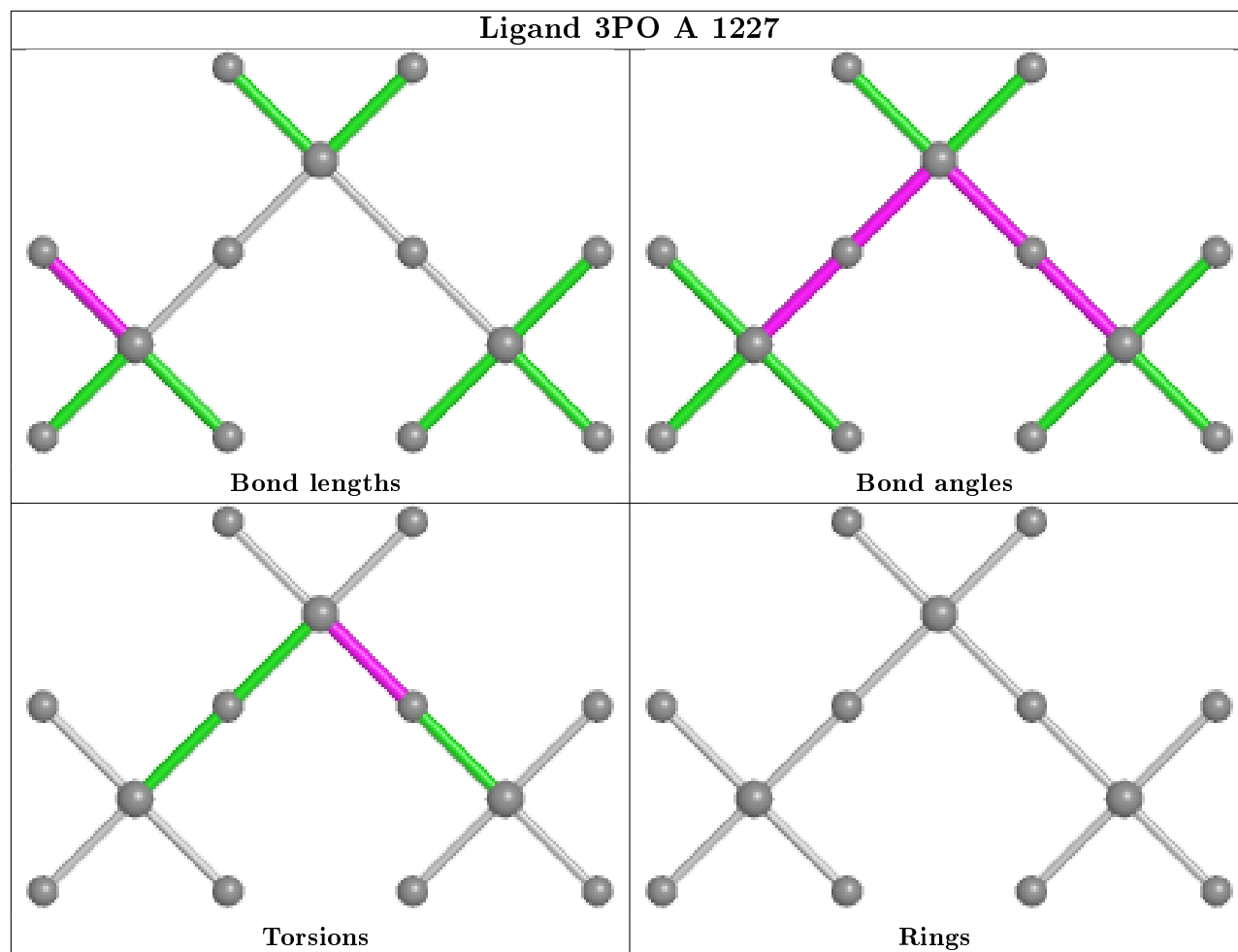
All (2) torsion outliers are listed below:

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.