Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 10:36 PM EDT

PDB ID	:	3P5R
Title	:	Crystal Structure of Taxadiene Synthase from Pacific Yew (Taxus brevifolia) in complex with Mg2+ and 2-fluorogeranylgeranyl diphosphate
Authors	:	Koksal, M.; Christianson, D.W.
Deposited on	:	2010-10-10
Resolution	:	2.25 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:

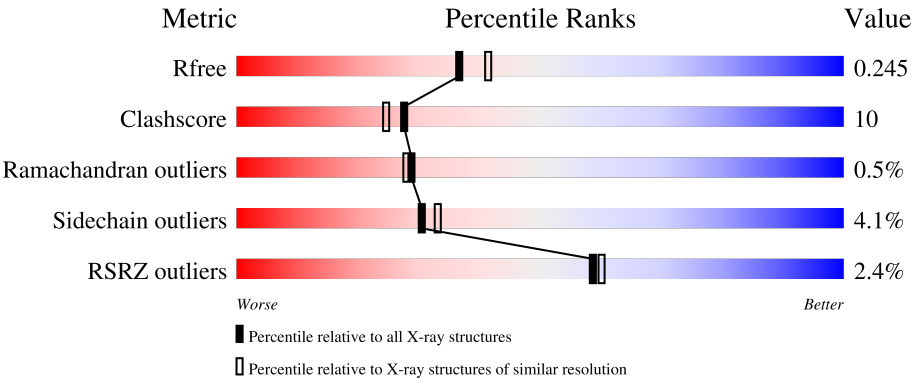
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 <=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	764	4% 75% 21%
1	B	764	% 75% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13321 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 Taxadiene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	4	0
			6078	3881	1022	1141	34			
1	B	738	Total	C	N	O	S	0	4	0
			5971	3812	999	1126	34			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	MET	-	initiating methionine	UNP Q41594
A	863	GLY	-	expression tag	UNP Q41594
A	864	SER	-	expression tag	UNP Q41594
A	865	HIS	-	expression tag	UNP Q41594
A	866	HIS	-	expression tag	UNP Q41594
A	867	HIS	-	expression tag	UNP Q41594
A	868	HIS	-	expression tag	UNP Q41594
A	869	HIS	-	expression tag	UNP Q41594
A	870	HIS	-	expression tag	UNP Q41594
B	107	MET	-	initiating methionine	UNP Q41594
B	863	GLY	-	expression tag	UNP Q41594
B	864	SER	-	expression tag	UNP Q41594
B	865	HIS	-	expression tag	UNP Q41594
B	866	HIS	-	expression tag	UNP Q41594
B	867	HIS	-	expression tag	UNP Q41594
B	868	HIS	-	expression tag	UNP Q41594
B	869	HIS	-	expression tag	UNP Q41594
B	870	HIS	-	expression tag	UNP Q41594

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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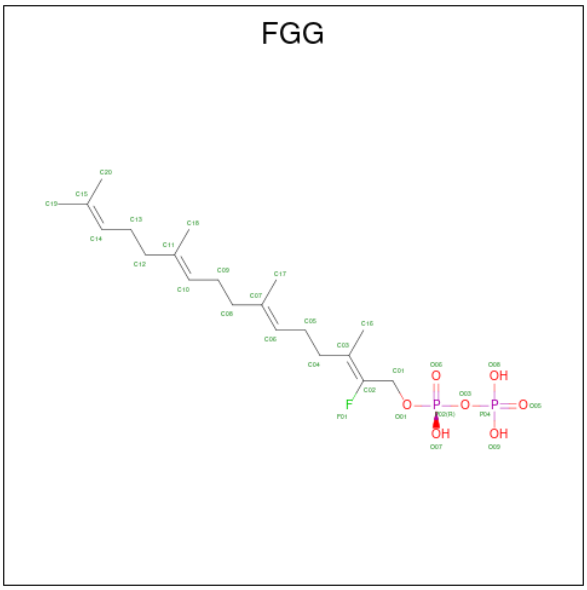
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0

- Molecule 3 is (2Z,6E,10E)-2-fluoro-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraen-1-yl trihydrogen diphosphate (three-letter code: FGG) (formula: $C_{20}H_{35}FO_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F O P 30 20 1 7 2	0	0
3	B	1	Total C F O P 30 20 1 7 2	0	0

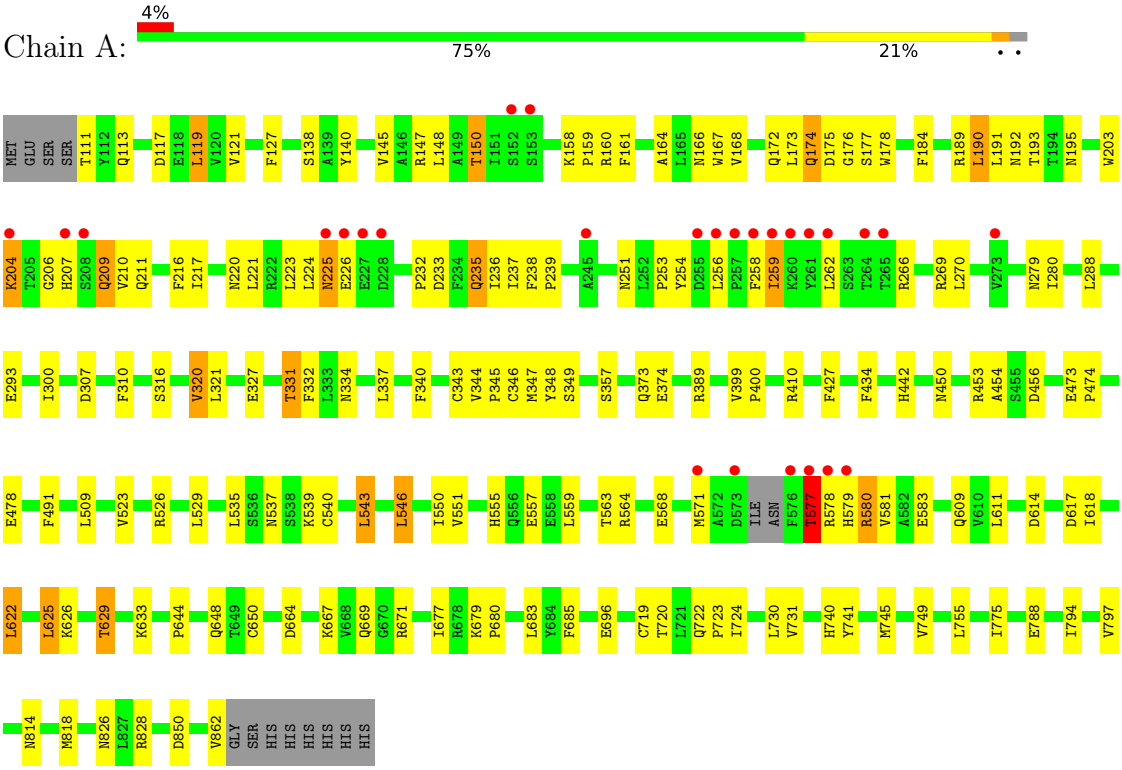
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	569	Total O 569 569	0	0
4	B	637	Total O 637 637	0	0

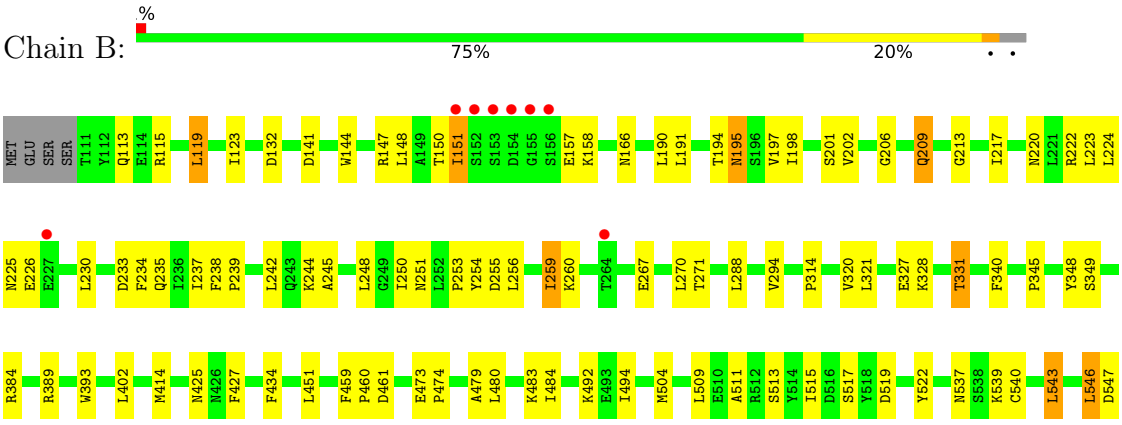
3 Residue-property plots (i)

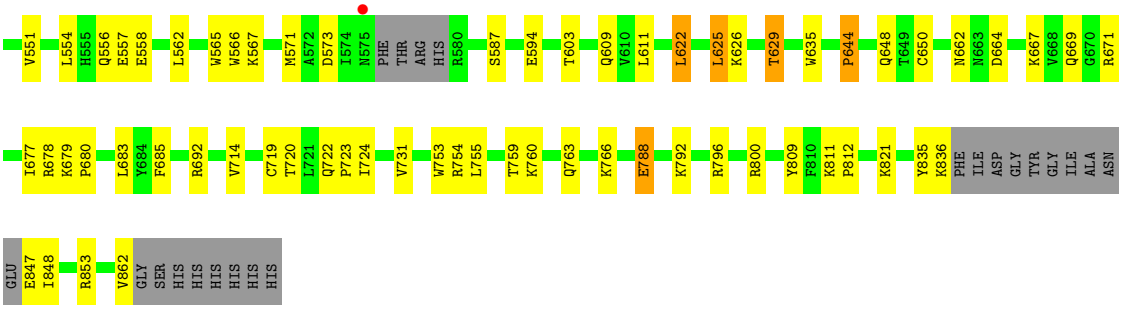
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Taxadiene synthase



• Molecule 1: Taxadiene synthase




V551
L554
H555
Q556
E557
E558
L562
W565
W566
K567
M571
A572
D573
I574
N575
PHE
THR
ARG
HIS
R580
S587
E594
T603
Q609
V610
L611
L622
L625
K626
T629
W635
P644
Q648
T649
C650
N662
N663
D664
K667
V668
Q669
G670
R671
I677
R678
K679
P680
L683
Y684
F685
R692
V714
C719
T720
L721
Q722
P723
I724
V731
W753
R754
L755
T759
K760
Q763
K766
E788
K792
R796
R800
Y809
F810
K811
P812
K821
Y835
K836
PHE
ILE
ASP
GLY
TYR
GLY
ILE
ALA
ASN
GLU
E847
I848
R853
V862
GLY
SER
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.05Å 201.98Å 81.43Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	43.41 – 2.25 43.41 – 2.25	Depositor EDS
% Data completeness (in resolution range)	81.0 (43.41-2.25) 81.0 (43.41-2.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.187 , 0.250 0.183 , 0.245	Depositor DCC
R_{free} test set	2014 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13321	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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	0.31	0/6239	0.45	0/8448
1	B	0.31	0/6127	0.46	0/8297
All	All	0.31	0/12366	0.45	0/16745

There are no bond length outliers.

There are no bond angle outliers.

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	6078	0	5956	121	0
1	B	5971	0	5854	112	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	30	0	32	7	0
3	B	30	0	32	7	0
4	A	569	0	0	7	0
4	B	637	0	0	8	0
All	All	13321	0	11874	241	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 10.

All (241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:MET:HE1	1:B:650:CYS:HA	1.50	0.94
1:A:175:ASP:N	1:A:176:GLY:HA2	1.81	0.93
1:A:669:GLN:HE22	1:A:731:VAL:H	1.24	0.86
1:B:254:TYR:HA	1:B:259:ILE:HD11	1.58	0.84
1:A:609:GLN:HE22	1:A:719:CYS:HB3	1.43	0.84
1:B:669:GLN:HE22	1:B:731:VAL:H	1.23	0.83
3:A:911:FGG:H17A	3:A:911:FGG:H04	1.60	0.83
1:A:850:ASP:HB2	4:A:1193:HOH:O	1.78	0.82
3:B:911:FGG:H17A	3:B:911:FGG:H04	1.62	0.82
1:B:151:ILE:HG12	1:B:157:GLU:HG2	1.64	0.80
1:A:537:ASN:HD22	1:A:540:CYS:H	1.30	0.79
1:B:609:GLN:HE22	1:B:719:CYS:HB3	1.48	0.77
1:B:340:PHE:CZ	1:B:345:PRO:HG3	2.19	0.77
1:A:225:ASN:HD22	1:A:225:ASN:H	1.32	0.76
1:A:221:LEU:HD12	1:A:253:PRO:HD2	1.69	0.75
1:A:256:LEU:HB2	1:A:259:ILE:HG22	1.67	0.75
1:B:629:THR:HB	1:B:685:PHE:HB3	1.69	0.74
1:A:629:THR:HB	1:A:685:PHE:HB3	1.73	0.71
1:A:577:THR:HG22	1:A:578:ARG:H	1.54	0.71
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.56	0.70
1:B:327:GLU:O	1:B:331:THR:HG22	1.93	0.69
1:A:150:THR:HG23	1:A:158:LYS:HG3	1.74	0.69
1:B:625:LEU:O	1:B:629:THR:HG23	1.92	0.69
1:A:664:ASP:HA	1:A:667:LYS:HE3	1.75	0.68
1:B:148:LEU:HD13	1:B:321:LEU:HD23	1.75	0.68
1:B:546:LEU:HD11	1:B:862:VAL:HG11	1.76	0.67
1:A:207:HIS:O	1:A:211:GLN:HG2	1.95	0.67
1:B:473:GLU:HB3	1:B:474:PRO:HD3	1.77	0.67
1:A:206:GLY:O	1:A:209:GLN:HG2	1.95	0.66
1:B:853:ARG:HD2	4:B:988:HOH:O	1.95	0.66
1:B:760:LYS:HG2	1:B:835:TYR:HB3	1.77	0.66
3:A:911:FGG:H16B	4:A:1182:HOH:O	1.95	0.66
1:A:119:LEU:HB3	1:A:543:LEU:HG	1.78	0.66
1:A:145:VAL:HG11	1:A:337:LEU:HD11	1.78	0.65
1:A:797:VAL:HA	4:A:1074:HOH:O	1.97	0.65
1:B:571:MET:CE	1:B:650:CYS:HA	2.26	0.65
1:A:580[B]:ARG:HH21	3:A:911:FGG:H19B	1.63	0.64
1:B:622:LEU:HD22	1:B:626:LYS:HE3	1.80	0.64
1:A:117:ASP:O	1:A:121:VAL:HG23	1.98	0.63
1:A:238:PHE:HB3	1:A:239:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ASN:HD21	1:A:539:LYS:HB2	1.63	0.63
1:B:233:ASP:O	1:B:237:ILE:HG12	1.98	0.63
1:B:242:LEU:HD13	1:B:259:ILE:HD12	1.80	0.63
1:B:511:ALA:O	1:B:515:ILE:HG13	1.99	0.62
1:A:644:PRO:O	1:A:648:GLN:HG3	1.99	0.61
1:A:720:THR:O	1:A:724:ILE:HG12	1.99	0.61
1:B:625:LEU:HD12	1:B:692:ARG:HG3	1.83	0.60
1:B:235:GLN:CD	1:B:235:GLN:H	2.04	0.60
1:A:563:THR:OG1	1:A:578:ARG:HG3	2.01	0.60
1:B:792:LYS:O	1:B:796:ARG:HG2	2.02	0.60
1:A:280:ILE:HG21	1:A:300:ILE:HD13	1.84	0.59
1:A:177:SER:HB3	1:A:216:PHE:CE1	2.37	0.59
3:A:911:FGG:H04	3:A:911:FGG:C17	2.33	0.58
1:B:609:GLN:NE2	1:B:719:CYS:HB3	2.18	0.58
1:A:225:ASN:HD22	1:A:225:ASN:N	2.00	0.58
1:A:473:GLU:HB3	1:A:474:PRO:HD3	1.85	0.58
1:A:327:GLU:O	1:A:331:THR:HG22	2.03	0.58
1:A:826:ASN:HD22	1:A:828:ARG:HH12	1.50	0.57
1:B:611:LEU:HD21	1:B:650:CYS:SG	2.45	0.57
1:B:194:THR:O	1:B:198:ILE:HG13	2.04	0.57
1:B:609:GLN:HB3	3:B:911:FGG:H17B	1.87	0.57
1:B:238:PHE:HB3	1:B:239:PRO:HD3	1.86	0.56
1:A:340:PHE:CZ	1:A:345:PRO:HG3	2.40	0.56
1:A:453:ARG:O	1:A:456:ASP:HB2	2.06	0.56
1:B:198:ILE:O	1:B:202:VAL:HG23	2.06	0.56
1:B:537:ASN:HD22	1:B:540:CYS:H	1.52	0.56
1:B:222:ARG:HG2	1:B:256:LEU:HD11	1.87	0.55
1:B:587:SER:OG	3:B:911:FGG:H13	2.05	0.55
1:A:579:HIS:O	1:A:583:GLU:HG3	2.06	0.55
1:A:178:TRP:CE3	1:A:193:THR:HG23	2.42	0.55
1:B:609:GLN:CB	3:B:911:FGG:H17B	2.36	0.55
3:B:911:FGG:H04	3:B:911:FGG:C17	2.35	0.55
1:B:141:ASP:HB3	1:B:314:PRO:HB2	1.87	0.55
1:B:206:GLY:O	1:B:209:GLN:HG2	2.07	0.55
1:B:755:LEU:O	1:B:759:THR:HG23	2.07	0.55
1:B:847:GLU:HG2	1:B:848:ILE:H	1.72	0.55
1:B:788:GLU:HG2	1:B:792:LYS:HZ3	1.72	0.54
1:A:614:ASP:O	1:A:618:ILE:HB	2.07	0.54
1:B:644:PRO:O	1:B:648:GLN:HG3	2.07	0.54
1:A:220:ASN:HA	1:A:223:LEU:HD13	1.90	0.53
1:A:340:PHE:CE1	1:A:345:PRO:HG3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:SER:HB2	1:A:346[A]:CYS:SG	2.48	0.53
1:A:571:MET:HE1	1:A:650:CYS:HA	1.90	0.53
1:A:113:GLN:OE1	1:A:550:ILE:HD13	2.09	0.53
1:A:389:ARG:HA	1:A:389:ARG:NE	2.23	0.53
1:A:450:ASN:ND2	1:A:453:ARG:HH11	2.07	0.53
1:B:414:MET:O	1:B:414:MET:HG3	2.09	0.53
1:B:847:GLU:HG2	1:B:848:ILE:N	2.24	0.53
1:A:178:TRP:CZ3	1:A:193:THR:HG23	2.43	0.52
1:A:622:LEU:HD22	1:A:626:LYS:HE3	1.92	0.52
1:A:225:ASN:N	1:A:225:ASN:ND2	2.57	0.52
1:B:267:GLU:O	1:B:271:THR:HG23	2.09	0.52
1:B:562:LEU:HD13	1:B:603:THR:HG21	1.92	0.52
1:B:788:GLU:CD	1:B:792:LYS:HZ1	2.12	0.52
1:B:519:ASP:HB3	1:B:522:TYR:HB2	1.92	0.51
1:A:609:GLN:NE2	1:A:719:CYS:HB3	2.20	0.51
1:A:347:MET:HE2	1:A:526:ARG:HD3	1.92	0.51
1:B:220:ASN:HA	1:B:223:LEU:HD12	1.92	0.51
1:A:175:ASP:N	1:A:176:GLY:CA	2.65	0.51
1:A:537:ASN:ND2	1:A:540:CYS:H	2.04	0.51
1:A:177:SER:HB3	1:A:216:PHE:CD1	2.46	0.51
1:A:316:SER:O	1:A:320:VAL:HG12	2.10	0.51
1:A:357:SER:CB	1:A:535:LEU:HD22	2.41	0.51
1:A:217:ILE:O	1:A:221:LEU:HG	2.12	0.50
1:B:402:LEU:HD11	1:B:451:LEU:HD13	1.93	0.50
1:A:148:LEU:CD1	1:A:321:LEU:HD23	2.41	0.50
1:A:254:TYR:HA	1:A:259:ILE:HD13	1.93	0.50
1:A:551:VAL:HG12	1:A:555:HIS:CE1	2.47	0.50
1:B:288:LEU:C	1:B:288:LEU:HD23	2.33	0.49
1:B:567:LYS:NZ	1:B:567:LYS:HB3	2.26	0.49
1:B:504:MET:CE	1:B:836:LYS:HD3	2.42	0.49
1:B:151:ILE:HA	1:B:157:GLU:HA	1.95	0.49
1:B:557:GLU:HG3	4:B:1058:HOH:O	2.13	0.49
1:B:714:VAL:HG21	1:B:753:TRP:HB3	1.93	0.49
1:A:224:LEU:HB3	1:A:258:PHE:CE2	2.48	0.49
1:B:314:PRO:HG2	1:B:345:PRO:O	2.12	0.49
1:B:460:PRO:O	1:B:461:ASP:HB2	2.13	0.49
1:B:546:LEU:CD1	1:B:862:VAL:HG11	2.43	0.49
1:A:307:ASP:O	1:A:332:PHE:HB2	2.12	0.49
1:A:622:LEU:CD2	1:A:626:LYS:HE3	2.43	0.49
1:A:474:PRO:O	1:A:478:GLU:HB2	2.13	0.49
1:A:826:ASN:ND2	1:A:828:ARG:HH12	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PHE:O	1:A:434:PHE:HA	2.13	0.48
1:A:679:LYS:HB2	1:A:680:PRO:HD3	1.95	0.48
1:A:161:PHE:HE1	1:A:334:ASN:HD22	1.62	0.48
1:A:814:ASN:OD1	1:B:425:ASN:HB3	2.13	0.48
1:B:679:LYS:HB2	1:B:680:PRO:HD3	1.95	0.48
1:A:755:LEU:HB3	1:A:794:ILE:HG23	1.95	0.48
1:B:213:GLY:O	1:B:217:ILE:HG13	2.13	0.48
1:A:357:SER:HB2	1:A:535:LEU:HD22	1.95	0.47
1:B:763:GLN:HG3	4:B:992:HOH:O	2.13	0.47
1:B:242:LEU:O	1:B:245:ALA:HB3	2.15	0.47
1:A:148:LEU:HD13	1:A:321:LEU:HD23	1.95	0.47
1:A:722:GLN:HB2	1:A:723:PRO:HD3	1.95	0.47
1:B:148:LEU:CD1	1:B:321:LEU:HD23	2.44	0.47
3:A:911:FGG:H16	3:A:911:FGG:H05A	1.56	0.47
1:A:625:LEU:O	1:A:629:THR:HG23	2.14	0.47
1:A:818:MET:HE1	4:A:1047:HOH:O	2.13	0.47
1:A:239:PRO:HB2	1:A:266:ARG:HD2	1.97	0.47
1:B:788:GLU:HB2	4:B:1105:HOH:O	2.14	0.47
1:A:167:TRP:CD1	1:A:343:CYS:HB3	2.50	0.47
1:B:664:ASP:HA	1:B:667:LYS:HE3	1.97	0.47
1:A:147:ARG:HH11	1:A:195:ASN:HD21	1.63	0.46
1:A:788:GLU:HG2	4:A:885:HOH:O	2.15	0.46
1:B:113:GLN:HA	1:B:113:GLN:NE2	2.30	0.46
1:A:288:LEU:C	1:A:288:LEU:HD23	2.35	0.46
1:B:115:ARG:HH22	1:B:862:VAL:HG12	1.81	0.46
1:B:119:LEU:HB3	1:B:543:LEU:HG	1.96	0.46
3:B:911:FGG:H17	3:B:911:FGG:H09	1.78	0.46
1:A:279:ASN:CG	1:A:280:ILE:H	2.19	0.46
1:A:150:THR:HG22	1:A:160:ARG:HA	1.97	0.46
1:B:754:ARG:O	1:B:754:ARG:HD3	2.15	0.46
1:B:720:THR:O	1:B:724:ILE:HG12	2.15	0.46
1:A:235:GLN:HB3	1:A:262:LEU:HD22	1.98	0.46
1:B:132:ASP:HB3	1:B:348:TYR:CE1	2.50	0.46
1:A:111:THR:N	4:A:1158:HOH:O	2.49	0.46
1:A:740:HIS:CG	1:A:741:TYR:H	2.32	0.46
1:A:357:SER:HB2	1:A:535:LEU:CD2	2.46	0.45
1:A:571:MET:CE	1:A:650:CYS:HA	2.46	0.45
1:A:204:LYS:HD2	1:A:204:LYS:HA	1.64	0.45
1:A:745:MET:O	1:A:749:VAL:HG23	2.16	0.45
1:B:147:ARG:HH11	1:B:195:ASN:HD21	1.65	0.45
1:B:197:VAL:CG1	1:B:250:ILE:HD13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:MET:HE2	1:B:836:LYS:HD3	1.98	0.45
1:A:174:GLN:C	1:A:176:GLY:HA2	2.37	0.45
1:B:197:VAL:HG12	1:B:250:ILE:HD13	1.99	0.45
1:A:677:ILE:O	1:A:680:PRO:HD2	2.16	0.45
1:B:340:PHE:CE1	1:B:345:PRO:HG3	2.50	0.45
1:B:348:TYR:CG	1:B:349:SER:HA	2.51	0.45
1:B:504:MET:HE1	1:B:836:LYS:HB2	1.99	0.45
1:A:190:LEU:HD12	1:A:190:LEU:HA	1.83	0.45
1:A:232:PRO:HB3	1:A:442:HIS:CE1	2.52	0.45
1:A:236:ILE:HD11	1:A:269:ARG:NH1	2.32	0.45
1:B:150:THR:HG23	1:B:158:LYS:HG3	1.98	0.45
1:A:410:ARG:HB2	1:A:454:ALA:HA	1.99	0.44
1:A:206:GLY:O	1:A:210:VAL:HG23	2.17	0.44
1:A:546:LEU:HD12	1:A:862:VAL:HG21	1.98	0.44
1:B:328:LYS:HE2	1:B:328:LYS:HB3	1.82	0.44
1:A:564:ARG:HD2	1:A:568:GLU:OE2	2.16	0.44
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.81	0.44
1:B:800:ARG:HG2	4:B:1235:HOH:O	2.16	0.44
1:A:622:LEU:HD12	1:A:696:GLU:OE2	2.17	0.44
1:B:662:ASN:ND2	1:B:677:ILE:HD13	2.33	0.44
1:A:233:ASP:O	1:A:237:ILE:HG12	2.17	0.44
1:A:633:LYS:HB2	1:A:633:LYS:NZ	2.32	0.44
1:B:389:ARG:NE	1:B:389:ARG:HA	2.32	0.44
1:B:719:CYS:O	1:B:723:PRO:HG2	2.18	0.44
1:B:547:ASP:O	1:B:551:VAL:HG23	2.18	0.43
1:B:259:ILE:O	1:B:259:ILE:HG13	2.16	0.43
1:B:484:ILE:HD13	1:B:494:ILE:HD12	2.00	0.43
1:A:559:LEU:HB3	1:A:578:ARG:HH21	1.84	0.43
1:B:384:ARG:NH1	4:B:1032:HOH:O	2.52	0.43
1:B:226:GLU:HG3	4:B:1076:HOH:O	2.19	0.43
1:B:255:ASP:O	1:B:260:LYS:HD3	2.19	0.43
1:A:348:TYR:CG	1:A:349:SER:HA	2.54	0.42
1:A:184:PHE:CE2	1:A:189:ARG:HG3	2.54	0.42
3:A:911:FGG:C17	3:A:911:FGG:C04	2.97	0.42
1:A:270:LEU:HD13	1:A:293:GLU:OE2	2.18	0.42
1:A:633:LYS:HB2	1:A:633:LYS:HZ3	1.84	0.42
1:B:244:LYS:HD2	1:B:244:LYS:HA	1.85	0.42
1:A:775:ILE:N	1:A:775:ILE:HD12	2.35	0.42
1:B:253:PRO:HB2	1:B:256:LEU:HG	2.01	0.42
1:A:164:ALA:O	1:A:168:VAL:HG23	2.20	0.41
1:B:270:LEU:O	1:B:294:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ASN:HD21	1:B:539:LYS:HB2	1.85	0.41
1:A:225:ASN:HA	1:A:226:GLU:HA	1.68	0.41
1:B:479:ALA:HA	1:B:483:LYS:HG2	2.02	0.41
1:A:159:PRO:HA	1:A:203:TRP:CZ2	2.55	0.41
1:A:491:PHE:CD2	1:A:491:PHE:C	2.94	0.41
1:B:150:THR:O	1:B:151:ILE:C	2.59	0.41
1:B:504:MET:HB2	1:B:504:MET:HE3	1.92	0.41
1:A:225:ASN:H	1:A:225:ASN:ND2	2.06	0.41
1:B:484:ILE:CD1	1:B:494:ILE:HD12	2.51	0.41
1:B:554:LEU:O	1:B:558:GLU:HG3	2.20	0.41
1:A:172:GLN:OE1	1:A:209:GLN:HB3	2.19	0.41
1:A:140:TYR:HB2	1:A:192:ASN:OD1	2.21	0.41
1:B:427:PHE:O	1:B:434:PHE:HA	2.20	0.41
1:B:480:LEU:HD21	1:B:494:ILE:HB	2.02	0.41
1:B:722:GLN:HB2	1:B:723:PRO:HD3	2.02	0.41
3:B:911:FGG:H05A	3:B:911:FGG:H16	1.65	0.41
1:A:344:VAL:HA	1:A:345:PRO:HD3	1.88	0.41
1:A:523:VAL:HG21	1:A:529:LEU:HB3	2.03	0.41
3:A:911:FGG:H20B	3:A:911:FGG:H12A	2.03	0.41
1:B:123:ILE:HD12	1:B:543:LEU:HD12	2.02	0.41
1:B:201:SER:HB2	1:B:248:LEU:HD13	2.02	0.41
1:B:556:GLN:NE2	4:B:886:HOH:O	2.54	0.41
1:B:565:TRP:CZ3	1:B:566:TRP:HE3	2.39	0.41
1:B:811:LYS:HA	1:B:812:PRO:HD3	1.94	0.41
1:A:617:ASP:OD1	1:A:618:ILE:HG13	2.20	0.40
1:B:459:PHE:HB3	1:B:460:PRO:CD	2.52	0.40
1:B:809:TYR:HA	1:B:821:LYS:HE2	2.03	0.40
1:A:178:TRP:CE3	1:A:193:THR:HA	2.56	0.40
1:B:759:THR:OG1	1:B:760:LYS:HD3	2.20	0.40
1:A:310:PHE:CE2	1:A:320:VAL:HG11	2.56	0.40
1:A:399:VAL:HA	1:A:400:PRO:HD3	1.89	0.40
1:A:730:LEU:HB3	1:B:389:ARG:HD2	2.03	0.40
1:A:127:PHE:CG	1:A:374:GLU:HB3	2.57	0.40
1:A:578:ARG:NE	4:A:1299:HOH:O	2.55	0.40
1:B:230:LEU:HD22	1:B:234:PHE:CD1	2.57	0.40
1:B:635:TRP:CE3	1:B:678:ARG:HG2	2.56	0.40
1:B:254:TYR:HA	1:B:259:ILE:CD1	2.40	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	750/764 (98%)	712 (95%)	35 (5%)	3 (0%)	34	35
1	B	736/764 (96%)	701 (95%)	31 (4%)	4 (0%)	29	28
All	All	1486/1528 (97%)	1413 (95%)	66 (4%)	7 (0%)	29	28

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	LEU
1	B	151	ILE
1	A	204	LYS
1	B	225	ASN
1	B	224	LEU
1	A	577	THR
1	B	644	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	665/674 (99%)	637 (96%)	28 (4%)	30	32
1	B	656/674 (97%)	629 (96%)	27 (4%)	30	33
All	All	1321/1348 (98%)	1266 (96%)	55 (4%)	30	32

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	150	THR
1	A	166	ASN
1	A	174	GLN
1	A	190	LEU
1	A	191	LEU
1	A	209	GLN
1	A	225	ASN
1	A	235	GLN
1	A	251	ASN
1	A	259	ILE
1	A	320	VAL
1	A	331	THR
1	A	373	GLN
1	A	509	LEU
1	A	543	LEU
1	A	546	LEU
1	A	557	GLU
1	A	577	THR
1	A	580[A]	ARG
1	A	580[B]	ARG
1	A	581	VAL
1	A	611	LEU
1	A	622	LEU
1	A	625	LEU
1	A	629	THR
1	A	671	ARG
1	A	683	LEU
1	B	119	LEU
1	B	144	TRP
1	B	166	ASN
1	B	190	LEU
1	B	191	LEU
1	B	195	ASN
1	B	209	GLN
1	B	251	ASN
1	B	259	ILE
1	B	320	VAL
1	B	331	THR
1	B	393	TRP
1	B	492	LYS
1	B	509	LEU
1	B	513	SER

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Mol	Chain	Res	Type
1	B	517	SER
1	B	543	LEU
1	B	546	LEU
1	B	573	ASP
1	B	594	GLU
1	B	622	LEU
1	B	625	LEU
1	B	629	THR
1	B	671	ARG
1	B	683	LEU
1	B	766	LYS
1	B	788	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	174	GLN
1	A	183	HIS
1	A	195	ASN
1	A	207	HIS
1	A	212	GLN
1	A	220	ASN
1	A	225	ASN
1	A	235	GLN
1	A	286	ASN
1	A	334	ASN
1	A	373	GLN
1	A	403	ASN
1	A	450	ASN
1	A	537	ASN
1	A	556	GLN
1	A	579	HIS
1	A	609	GLN
1	A	662	ASN
1	A	669	GLN
1	A	826	ASN
1	B	166	ASN
1	B	170	ASN
1	B	174	GLN
1	B	183	HIS
1	B	195	ASN

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Mol	Chain	Res	Type
1	B	212	GLN
1	B	220	ASN
1	B	251	ASN
1	B	286	ASN
1	B	298	ASN
1	B	334	ASN
1	B	403	ASN
1	B	450	ASN
1	B	537	ASN
1	B	556	GLN
1	B	609	GLN
1	B	662	ASN
1	B	669	GLN
1	B	826	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\#\|Z\|>2$
3	FGG	B	911	2	27,29,29	1.28	3 (11%)	30,39,39	1.59	6 (20%)
3	FGG	A	911	2	27,29,29	1.25	2 (7%)	30,39,39	1.46	8 (26%)

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	FGG	B	911	2	-	9/28/34/34	-
3	FGG	A	911	2	-	9/28/34/34	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	911	FGG	O01-C01	-3.84	1.40	1.43
3	A	911	FGG	F01-C02	-3.71	1.32	1.36
3	A	911	FGG	O01-C01	-3.59	1.40	1.43
3	B	911	FGG	F01-C02	-3.49	1.32	1.36
3	B	911	FGG	P04-O08	-2.01	1.47	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	911	FGG	C18-C11-C12	3.73	121.55	115.27
3	B	911	FGG	C09-C10-C11	-3.22	119.91	127.66
3	A	911	FGG	C18-C11-C12	2.95	120.23	115.27
3	B	911	FGG	C16-C03-C04	2.63	121.01	115.33
3	A	911	FGG	C09-C10-C11	-2.63	121.33	127.66
3	A	911	FGG	C20-C15-C19	2.52	120.17	114.60
3	B	911	FGG	P02-O03-P04	-2.46	124.38	132.83
3	B	911	FGG	C20-C15-C19	2.29	119.67	114.60
3	A	911	FGG	P02-O03-P04	-2.28	125.02	132.83
3	B	911	FGG	C05-C06-C07	-2.25	122.24	127.66
3	A	911	FGG	C16-C03-C04	2.16	119.99	115.33
3	A	911	FGG	C13-C14-C15	-2.12	120.51	127.75
3	A	911	FGG	C17-C07-C08	2.06	118.73	115.27
3	A	911	FGG	C05-C06-C07	-2.05	122.72	127.66

There are no chirality outliers.

All (18) torsion outliers are listed below:

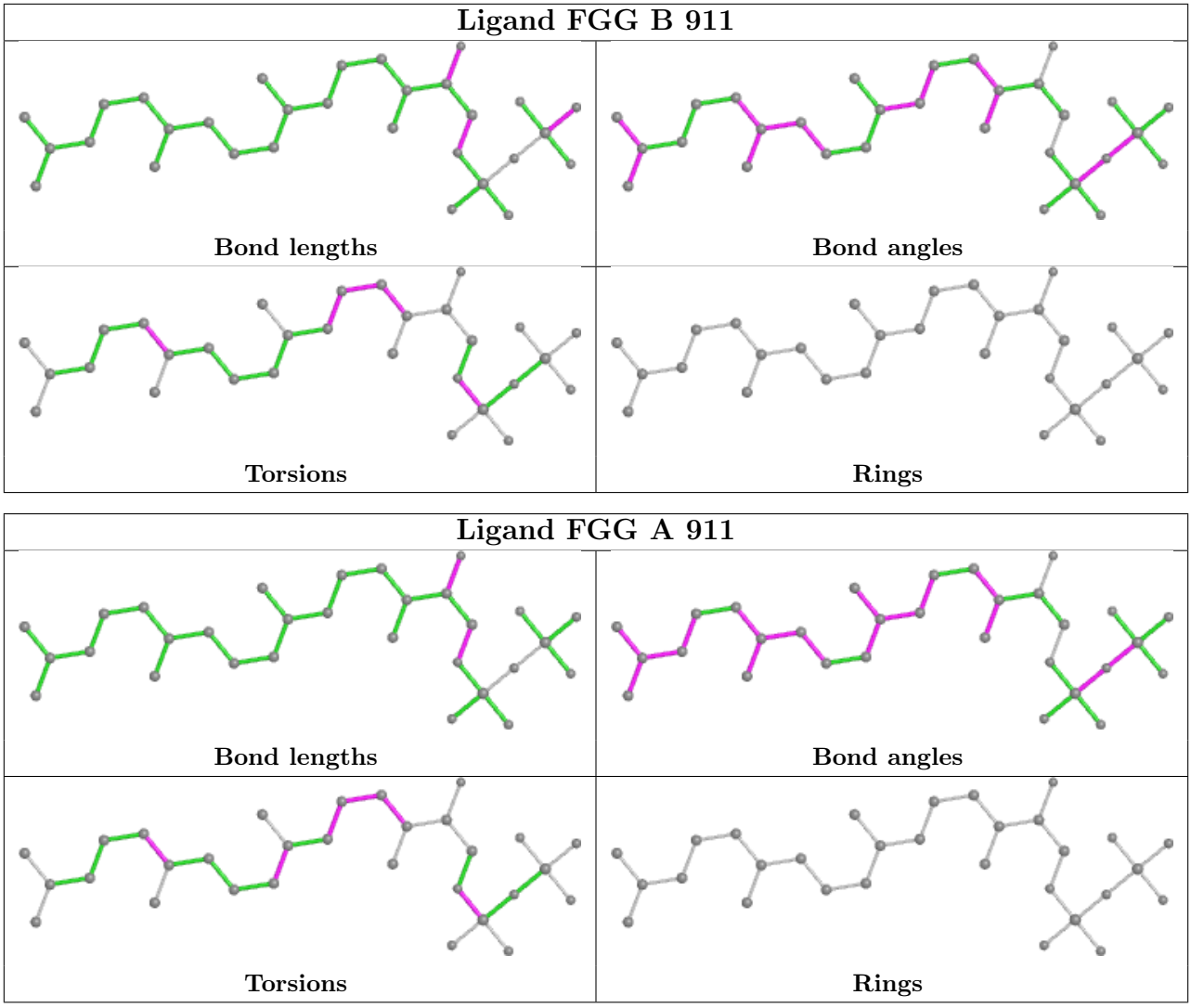
Mol	Chain	Res	Type	Atoms
3	A	911	FGG	C01-O01-P02-O03
3	A	911	FGG	C02-C03-C04-C05
3	B	911	FGG	C01-O01-P02-O03
3	B	911	FGG	C02-C03-C04-C05
3	B	911	FGG	C10-C11-C12-C13
3	B	911	FGG	C18-C11-C12-C13
3	A	911	FGG	C16-C03-C04-C05
3	B	911	FGG	C16-C03-C04-C05
3	A	911	FGG	C04-C05-C06-C07
3	A	911	FGG	C03-C04-C05-C06
3	B	911	FGG	C04-C05-C06-C07
3	A	911	FGG	C01-O01-P02-O06
3	A	911	FGG	C01-O01-P02-O07
3	B	911	FGG	C01-O01-P02-O06
3	A	911	FGG	C17-C07-C08-C09
3	B	911	FGG	C03-C04-C05-C06
3	B	911	FGG	C01-O01-P02-O07
3	A	911	FGG	C18-C11-C12-C13

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	911	FGG	7	0
3	A	911	FGG	7	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.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	750/764 (98%)	-0.16	27 (3%) 42 42	9, 19, 64, 128	0
1	B	738/764 (96%)	-0.31	9 (1%) 79 80	9, 18, 48, 113	0
All	All	1488/1528 (97%)	-0.23	36 (2%) 59 60	9, 18, 57, 128	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	153	SER	6.5
1	B	152	SER	4.9
1	A	152	SER	4.7
1	B	155	GLY	4.6
1	B	154	ASP	4.4
1	A	264	THR	3.9
1	B	227	GLU	3.9
1	A	227	GLU	3.8
1	A	258	PHE	3.7
1	A	579	HIS	3.7
1	A	577	THR	3.2
1	B	264	THR	3.2
1	A	273	VAL	3.1
1	A	578	ARG	3.0
1	A	257	PRO	3.0
1	A	226	GLU	2.9
1	A	260	LYS	2.9
1	B	575	ASN	2.8
1	A	225	ASN	2.8
1	A	153	SER	2.7
1	A	576	PHE	2.7
1	A	261	TYR	2.6
1	B	156	SER	2.6
1	A	259	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	151	ILE	2.4
1	A	245	ALA	2.4
1	A	571	MET	2.3
1	A	573	ASP	2.2
1	A	228	ASP	2.2
1	A	207	HIS	2.2
1	A	255	ASP	2.2
1	A	204	LYS	2.1
1	A	208	SER	2.1
1	A	262	LEU	2.1
1	A	265	THR	2.1
1	A	256	LEU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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.

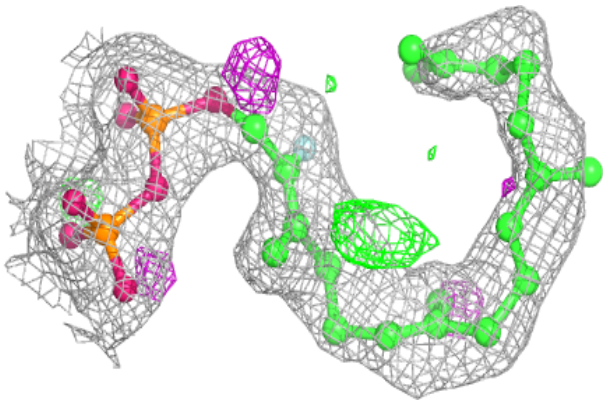
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	903	1/1	0.95	0.07	18,18,18,18	0
2	MG	A	903	1/1	0.97	0.08	13,13,13,13	0
2	MG	A	902	1/1	0.97	0.08	16,16,16,16	0
3	FGG	A	911	30/30	0.97	0.14	13,28,39,45	0
3	FGG	B	911	30/30	0.97	0.15	14,29,38,40	0
2	MG	A	901	1/1	0.99	0.14	13,13,13,13	0
2	MG	B	901	1/1	0.99	0.10	12,12,12,12	0
2	MG	B	902	1/1	0.99	0.09	12,12,12,12	0

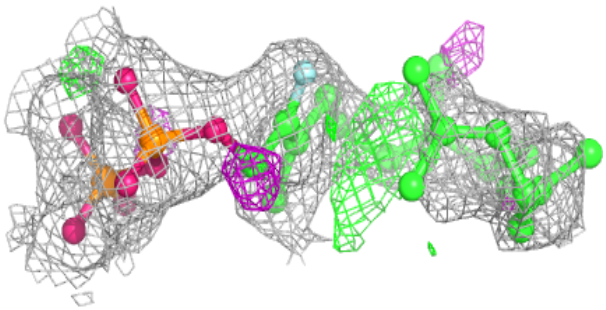
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

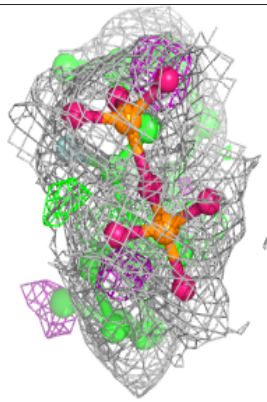
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FGG A 911:

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

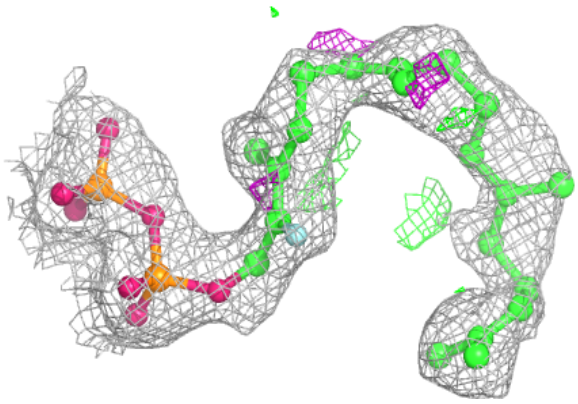


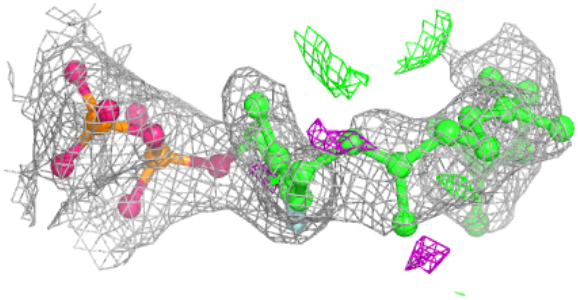


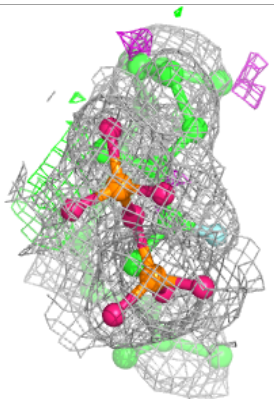


Electron density around FGG B 911:

$2mF_o$-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.