



Full wwPDB X-ray Structure Validation Report

May 13, 2020 – 07:19 pm BST

PDB ID : 5ZOI
Title : Crystal Structure of alpha1,3-Fucosyltransferase
Authors : Tan, Y.; Yang, G.
Deposited on : 2018-04-13
Resolution : 3.19 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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

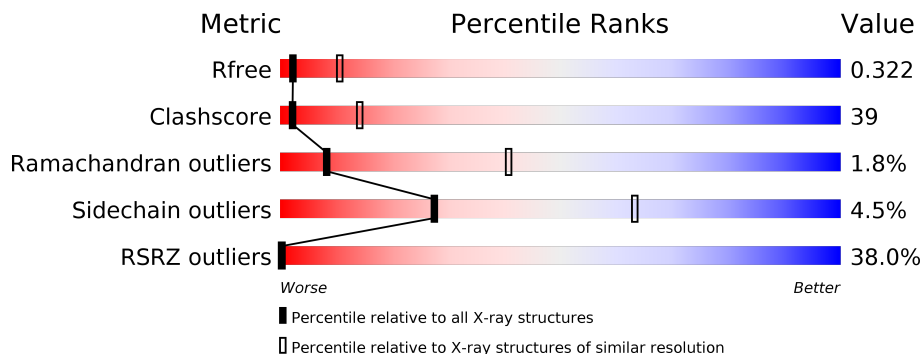
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C06	A	501	-	-	X	X
2	C06	B	501	-	-	X	X

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 5718 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 Alpha-(1,3)-fucosyltransferase FucT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	343	2821	1834	454	526	7	0	0	0
1	B	343	2821	1834	454	526	7	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

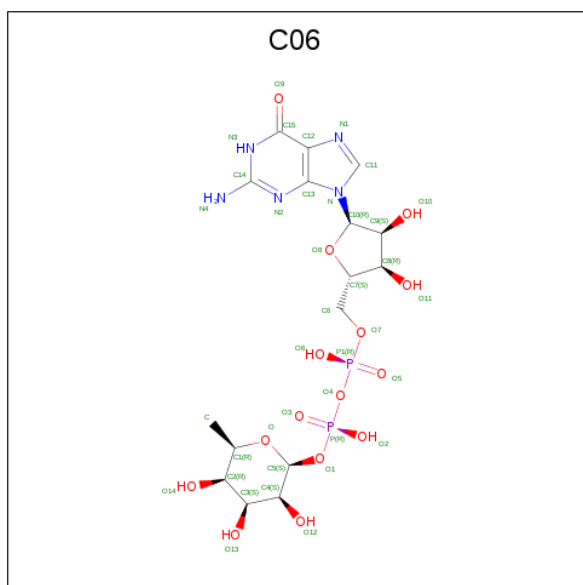
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	PHE	SER	engineered mutation	UNP O30511
A	127	ASN	ASP	engineered mutation	UNP O30511
A	128	GLU	ARG	engineered mutation	UNP O30511
A	131	ILE	HIS	engineered mutation	UNP O30511
A	199	ASN	TYR	engineered mutation	UNP O30511
A	340	ASP	GLU	engineered mutation	UNP O30511
A	368	ALA	VAL	engineered mutation	UNP O30511
A	413	LEU	-	expression tag	UNP O30511
A	414	GLU	-	expression tag	UNP O30511
A	415	HIS	-	expression tag	UNP O30511
A	416	HIS	-	expression tag	UNP O30511
A	417	HIS	-	expression tag	UNP O30511
A	418	HIS	-	expression tag	UNP O30511
A	419	HIS	-	expression tag	UNP O30511
A	420	HIS	-	expression tag	UNP O30511
B	45	PHE	SER	engineered mutation	UNP O30511
B	127	ASN	ASP	engineered mutation	UNP O30511
B	128	GLU	ARG	engineered mutation	UNP O30511
B	131	ILE	HIS	engineered mutation	UNP O30511
B	199	ASN	TYR	engineered mutation	UNP O30511
B	340	ASP	GLU	engineered mutation	UNP O30511
B	368	ALA	VAL	engineered mutation	UNP O30511
B	413	LEU	-	expression tag	UNP O30511
B	414	GLU	-	expression tag	UNP O30511
B	415	HIS	-	expression tag	UNP O30511

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Chain	Residue	Modelled	Actual	Comment	Reference
B	416	HIS	-	expression tag	UNP O30511
B	417	HIS	-	expression tag	UNP O30511
B	418	HIS	-	expression tag	UNP O30511
B	419	HIS	-	expression tag	UNP O30511
B	420	HIS	-	expression tag	UNP O30511

- Molecule 2 is [(2S,3R,4S,5R)-5-(2-azanyl-6-oxidanylidene-1H-purin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl [(2S,3S,4S,5R,6R)-6-methyl-3,4,5-tris(oxidanyl)oxan-2-yl] hydrogen phosphate (three-letter code: C06) (formula: C₁₆H₂₅N₅O₁₅P₂).

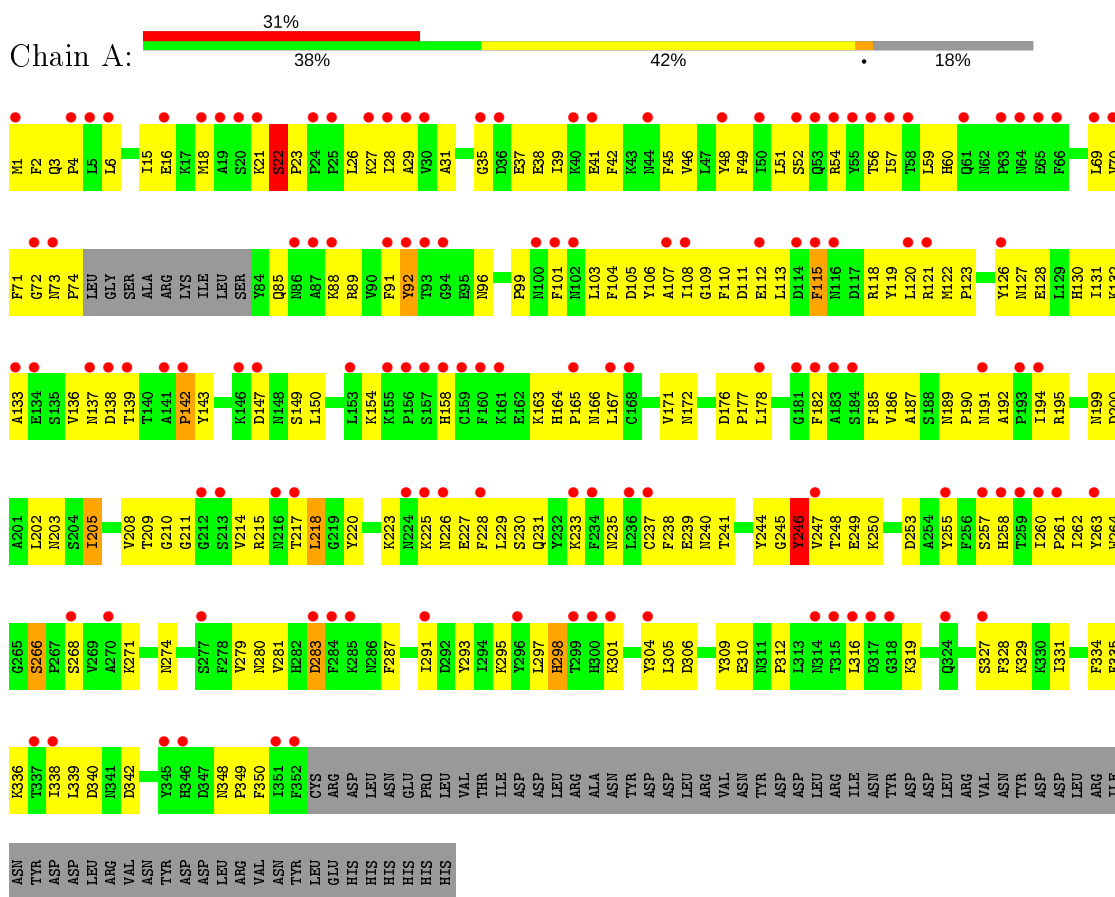


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total	C	N	O	P	0	0
			38	16	5	15	2		
2	B	1	Total	C	N	O	P	0	0
			38	16	5	15	2		

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: Alpha-(1,3)-fucosyltransferase FucT



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	121.66 Å 121.66 Å 64.72 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.80 – 3.19 39.82 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.80-3.19) 99.8 (39.82-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	250.53 (at 3.18 Å)	Xtrriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.287 , 0.316 0.308 , 0.322	Depositor DCC
R_{free} test set	1773 reflections (9.93%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtrriage
Anisotropy	0.098	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.084 for -h,-k,l 0.390 for h,-h-k,-l 0.085 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.435 for H, K, L 0.431 for K, H, -L 0.069 for -K, -H, -L 0.065 for -h,-k,l	Depositor
Outliers	0 of 17849 reflections	Xtrriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	5718	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1886e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C06

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	0.53	0/2907	0.66	0/3947
1	B	0.52	0/2907	0.68	2/3947 (0.1%)
All	All	0.52	0/5814	0.67	2/7894 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	GLN	CA-CB-CG	-7.19	97.58	113.40
1	B	271	LYS	CD-CE-NZ	5.29	123.86	111.70

There are no chirality outliers.

There are no planarity outliers.

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	2821	0	2695	220	0
1	B	2821	0	2694	223	1
2	A	38	0	0	33	0
2	B	38	0	0	56	0
All	All	5718	0	5389	437	1

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 39.

All (437) 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:42:PHE:HA	1:B:45:PHE:CE2	1.27	1.64
1:A:42:PHE:HA	1:A:45:PHE:CE2	1.36	1.58
1:A:195:ARG:HD3	2:A:501:C06:C	1.14	1.56
1:A:187:ALA:CB	1:A:195:ARG:HE	1.19	1.52
1:A:189:ASN:HB3	2:A:501:C06:C4	1.43	1.48
1:B:195:ARG:CD	2:B:501:C06:O3	1.64	1.44
1:B:42:PHE:CD1	1:B:45:PHE:HZ	1.38	1.40
1:A:192:ALA:HB3	2:A:501:C06:O14	1.21	1.34
1:B:189:ASN:HB3	2:B:501:C06:C4	1.56	1.33
1:B:192:ALA:CB	2:B:501:C06:O14	1.75	1.33
1:B:189:ASN:HB3	2:B:501:C06:C3	1.59	1.33
1:B:189:ASN:CB	2:B:501:C06:C4	2.07	1.31
1:B:42:PHE:CD1	1:B:45:PHE:CZ	2.19	1.30
1:B:189:ASN:HB3	2:B:501:C06:C2	1.58	1.30
1:A:195:ARG:CD	2:A:501:C06:C	2.07	1.29
1:A:187:ALA:CB	1:A:195:ARG:NE	1.98	1.26
1:A:41:GLU:O	1:A:45:PHE:CD2	1.91	1.23
1:B:42:PHE:CA	1:B:45:PHE:CE2	2.23	1.20
1:A:45:PHE:CB	1:A:127:ASN:HD21	1.56	1.18
1:A:195:ARG:NH2	1:A:238:PHE:O	1.78	1.17
1:B:250:LYS:HD2	2:B:501:C06:P1	1.85	1.17
1:B:195:ARG:NE	2:B:501:C06:O	1.77	1.16
1:B:192:ALA:HB3	2:B:501:C06:O14	1.02	1.16
1:A:42:PHE:CA	1:A:45:PHE:CE2	2.28	1.16
1:A:225:LYS:HD2	2:A:501:C06:O10	1.44	1.15
1:B:225:LYS:HZ2	2:B:501:C06:C9	1.59	1.15
1:A:187:ALA:HB2	1:A:195:ARG:NE	1.61	1.12
1:B:195:ARG:HD2	2:B:501:C06:O3	1.27	1.12
1:A:45:PHE:HB2	1:A:127:ASN:HD21	1.14	1.11
1:A:189:ASN:CB	2:A:501:C06:C4	2.29	1.10
1:B:189:ASN:CB	2:B:501:C06:C3	2.26	1.09
1:B:250:LYS:NZ	2:B:501:C06:O11	1.82	1.09
1:A:187:ALA:HB1	1:A:195:ARG:NE	1.66	1.07
1:A:195:ARG:HD3	2:A:501:C06:C1	1.84	1.07
1:A:45:PHE:HB2	1:A:127:ASN:ND2	1.70	1.05
1:B:225:LYS:NZ	2:B:501:C06:C9	2.20	1.05
1:A:239:GLU:HA	2:A:501:C06:O2	1.58	1.02
1:B:200:ASP:OD2	1:B:215:ARG:NH1	1.93	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:LYS:HD2	2:B:501:C06:O10	1.61	1.01
1:A:195:ARG:CD	2:A:501:C06:O	2.06	1.01
1:B:189:ASN:CB	2:B:501:C06:C2	2.38	1.01
1:A:189:ASN:HB3	2:A:501:C06:C3	1.91	1.00
1:A:187:ALA:HB2	1:A:195:ARG:CZ	1.91	1.00
1:A:42:PHE:HA	1:A:45:PHE:CZ	1.97	0.99
1:B:189:ASN:HB3	2:B:501:C06:C1	1.92	0.99
1:A:192:ALA:CB	2:A:501:C06:O14	2.11	0.99
1:A:192:ALA:HB2	2:A:501:C06:O13	1.62	0.99
1:A:187:ALA:HB1	1:A:195:ARG:HE	0.83	0.98
1:B:42:PHE:CA	1:B:45:PHE:HE2	1.71	0.97
1:A:89:ARG:NH1	1:A:103:LEU:O	1.97	0.97
1:A:41:GLU:O	1:A:45:PHE:HD2	1.42	0.96
1:B:189:ASN:HB2	2:B:501:C06:C4	1.96	0.96
1:B:42:PHE:HD1	1:B:45:PHE:CZ	1.69	0.95
1:B:127:ASN:O	1:B:131:ILE:HD12	1.67	0.94
1:B:189:ASN:CG	2:B:501:C06:C3	2.36	0.93
1:A:112:GLU:OE1	1:A:271:LYS:NZ	2.03	0.92
1:B:195:ARG:NE	2:B:501:C06:O3	2.03	0.92
1:B:225:LYS:NZ	2:B:501:C06:O10	2.03	0.91
1:A:248:THR:OG1	1:A:250:LYS:NZ	2.04	0.91
1:B:196:ASN:O	1:B:215:ARG:NH1	2.05	0.90
1:A:239:GLU:OE1	1:A:250:LYS:NZ	2.04	0.89
1:B:195:ARG:HE	2:B:501:C06:C1	1.85	0.89
1:A:200:ASP:OD1	1:A:215:ARG:NH1	2.05	0.89
1:B:240:ASN:HB3	2:B:501:C06:O13	1.73	0.89
1:B:89:ARG:NH1	1:B:103:LEU:O	2.06	0.89
1:A:194:ILE:HG22	1:A:238:PHE:CE2	2.09	0.88
1:B:46:VAL:HB	1:B:127:ASN:OD1	1.73	0.88
1:B:16:GLU:O	1:B:54:ARG:NH2	2.07	0.88
1:A:195:ARG:HD2	2:A:501:C06:O	1.74	0.87
1:B:41:GLU:O	1:B:45:PHE:CD2	2.26	0.87
1:A:187:ALA:HB2	1:A:195:ARG:NH1	1.90	0.86
1:A:238:PHE:O	2:A:501:C06:O3	1.92	0.86
1:A:46:VAL:N	1:A:127:ASN:OD1	2.07	0.86
1:B:225:LYS:NZ	2:B:501:C06:O11	2.08	0.86
1:A:335:PHE:O	1:A:339:LEU:HG	1.76	0.86
1:B:239:GLU:OE2	1:B:248:THR:OG1	1.93	0.86
1:A:42:PHE:HA	1:A:45:PHE:HE2	1.04	0.85
1:B:250:LYS:HD2	2:B:501:C06:O4	1.76	0.85
1:B:240:ASN:CB	2:B:501:C06:O13	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:HB3	1:A:107:ALA:HA	1.59	0.84
1:B:42:PHE:CE1	1:B:45:PHE:HZ	1.93	0.84
1:A:42:PHE:CA	1:A:45:PHE:HE2	1.80	0.84
1:B:189:ASN:O	2:B:501:C06:C2	2.26	0.84
1:B:195:ARG:HD3	2:B:501:C06:O3	1.74	0.84
1:B:225:LYS:CD	2:B:501:C06:O10	2.26	0.83
1:A:239:GLU:CA	2:A:501:C06:O2	2.26	0.83
1:A:45:PHE:HB3	1:A:127:ASN:HD21	1.40	0.82
1:B:49:PHE:HZ	1:B:154:LYS:HZ1	1.27	0.82
1:A:16:GLU:O	1:A:54:ARG:NH1	2.11	0.81
1:A:195:ARG:CD	2:A:501:C06:C1	2.49	0.81
1:A:88:LYS:NZ	1:A:342:ASP:OD1	2.13	0.80
1:B:225:LYS:CE	2:B:501:C06:O10	2.31	0.78
1:B:5:LEU:HD22	1:B:312:PRO:HG2	1.64	0.77
1:B:42:PHE:HA	1:B:45:PHE:HE2	0.94	0.77
1:B:127:ASN:O	1:B:131:ILE:CD1	2.31	0.77
1:B:138:ASP:OD1	1:B:140:THR:N	2.12	0.76
1:B:192:ALA:HB2	2:B:501:C06:O14	1.86	0.76
1:B:324:GLN:O	1:B:330:LYS:NZ	2.15	0.75
1:B:115:PHE:HB3	1:B:118:ARG:HB2	1.66	0.75
1:B:42:PHE:HA	1:B:45:PHE:CZ	2.15	0.75
1:B:45:PHE:HA	1:B:127:ASN:HD21	1.50	0.75
1:B:85:GLN:O	1:B:346:HIS:NE2	2.20	0.75
1:A:127:ASN:O	1:A:131:ILE:HB	1.86	0.74
1:A:112:GLU:OE2	1:A:244:TYR:HB3	1.86	0.74
1:B:168:CYS:O	1:B:172:ASN:ND2	2.19	0.74
1:B:46:VAL:N	1:B:127:ASN:OD1	2.21	0.74
1:B:3:GLN:OE1	1:B:6:LEU:HD22	1.87	0.74
1:A:45:PHE:CB	1:A:127:ASN:ND2	2.36	0.74
1:A:186:VAL:HG11	1:A:225:LYS:HG3	1.70	0.73
1:B:195:ARG:NE	2:B:501:C06:C	2.50	0.73
1:A:171:VAL:HG22	1:A:258:HIS:HB2	1.70	0.73
1:B:225:LYS:HZ1	2:B:501:C06:C8	2.01	0.73
1:B:189:ASN:OD1	2:B:501:C06:C3	2.35	0.73
1:B:42:PHE:HD1	1:B:45:PHE:CE2	2.06	0.73
1:B:42:PHE:CD1	1:B:45:PHE:CE2	2.76	0.73
1:A:128:GLU:OE2	1:A:253:ASP:OD1	2.05	0.72
1:B:341:ASN:OD1	1:B:345:TYR:OH	2.08	0.72
1:B:225:LYS:NZ	2:B:501:C06:C8	2.52	0.72
1:A:194:ILE:HG22	1:A:238:PHE:CD2	2.25	0.71
1:B:189:ASN:O	2:B:501:C06:C	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HD11	1:B:228:PHE:HE1	1.55	0.70
1:A:205:ILE:HG21	1:A:295:LYS:HD3	1.72	0.70
1:A:46:VAL:HG23	1:A:130:HIS:ND1	2.07	0.70
1:B:42:PHE:HA	1:B:45:PHE:CD2	2.17	0.69
1:A:194:ILE:HG22	1:A:238:PHE:HE2	1.54	0.69
1:B:250:LYS:NZ	2:B:501:C06:O7	2.14	0.69
1:B:233:LYS:HD3	1:B:298:HIS:HE1	1.58	0.69
1:B:189:ASN:O	2:B:501:C06:C1	2.41	0.69
1:B:186:VAL:HG11	1:B:225:LYS:HG3	1.75	0.69
1:A:185:PHE:N	1:A:209:THR:O	2.23	0.69
1:A:187:ALA:HB2	1:A:195:ARG:HH11	1.58	0.69
1:A:226:ASN:ND2	1:A:257:SER:OG	2.26	0.69
1:B:140:THR:HB	1:B:161:LYS:HB2	1.73	0.69
1:A:239:GLU:C	2:A:501:C06:O2	2.31	0.68
1:B:195:ARG:NH2	1:B:195:ARG:HB2	2.08	0.68
1:B:296:TYR:O	1:B:300:HIS:N	2.27	0.68
1:A:192:ALA:CB	2:A:501:C06:O13	2.41	0.67
1:A:336:LYS:HA	1:A:339:LEU:HD12	1.74	0.67
1:B:180:ARG:HB2	1:B:233:LYS:HG3	1.77	0.67
1:B:255:TYR:OH	1:B:277:SER:OG	2.10	0.67
1:B:128:GLU:HG3	1:B:249:GLU:HB2	1.76	0.66
1:B:41:GLU:O	1:B:45:PHE:HD2	1.77	0.66
1:B:218:LEU:HD11	1:B:228:PHE:CE1	2.30	0.66
1:B:295:LYS:O	1:B:299:THR:OG1	2.14	0.66
1:B:120:LEU:HD21	1:B:331:ILE:HG12	1.76	0.66
1:A:240:ASN:N	2:A:501:C06:O2	2.28	0.65
1:A:250:LYS:HE2	2:A:501:C06:O2	1.97	0.65
1:B:195:ARG:CD	2:B:501:C06:O	2.44	0.65
1:A:262:ILE:HA	1:A:279:VAL:HB	1.77	0.65
1:B:212:GLY:O	1:B:216:ASN:ND2	2.29	0.65
1:A:35:GLY:O	1:A:39:ILE:N	2.29	0.64
1:A:15:ILE:HA	1:A:329:LYS:NZ	2.13	0.64
1:A:195:ARG:NE	2:A:501:C06:O	2.31	0.64
1:B:194:ILE:HG22	1:B:238:PHE:CD2	2.31	0.64
1:A:240:ASN:HA	2:A:501:C06:O13	1.98	0.64
1:A:106:TYR:HB3	1:A:334:PHE:CZ	2.33	0.63
1:A:70:VAL:HB	1:A:89:ARG:HA	1.79	0.63
1:A:45:PHE:CE1	1:A:92:TYR:HE2	2.17	0.63
1:B:264:TRP:HD1	1:B:281:VAL:HB	1.62	0.63
1:A:185:PHE:HB3	1:A:210:GLY:HA2	1.81	0.63
1:A:194:ILE:CG2	1:A:238:PHE:HE2	2.11	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LYS:HA	1:B:332:LEU:HB2	1.80	0.63
1:A:163:LYS:HE3	1:B:163:LYS:HE2	1.81	0.62
1:A:127:ASN:O	1:A:131:ILE:HD13	1.99	0.62
1:A:240:ASN:HB3	2:A:501:C06:O12	1.99	0.62
1:A:99:PRO:HG2	1:A:119:TYR:HE2	1.63	0.62
1:A:106:TYR:HB3	1:A:334:PHE:HZ	1.65	0.62
1:B:337:THR:O	1:B:340:ASP:HB2	1.99	0.62
1:B:99:PRO:HD3	1:B:111:ASP:OD2	1.99	0.62
1:B:199:ASN:O	1:B:203:ASN:N	2.30	0.61
1:A:45:PHE:HB2	1:A:127:ASN:CG	2.20	0.61
1:A:195:ARG:HD2	2:A:501:C06:O3	2.01	0.60
1:B:189:ASN:C	2:B:501:C06:C2	2.69	0.60
1:A:194:ILE:CG2	1:A:238:PHE:CE2	2.83	0.60
1:B:193:PRO:O	1:B:197:ALA:N	2.32	0.60
1:B:111:ASP:N	1:B:119:TYR:OH	2.35	0.59
1:B:233:LYS:HD3	1:B:298:HIS:CE1	2.37	0.59
1:A:209:THR:HA	1:A:217:THR:HB	1.85	0.58
1:A:49:PHE:CG	1:A:130:HIS:HE1	2.22	0.58
1:A:41:GLU:O	1:A:45:PHE:CE2	2.53	0.58
1:B:305:LEU:O	1:B:309:TYR:N	2.32	0.58
1:A:29:ALA:HB3	1:A:70:VAL:HG22	1.85	0.58
1:B:16:GLU:OE2	1:B:16:GLU:N	2.34	0.57
1:A:231:GLN:OE1	1:B:37:GLU:OE2	2.22	0.57
1:A:240:ASN:CB	2:A:501:C06:O13	2.53	0.57
1:A:3:GLN:HE22	1:A:143:TYR:HA	1.68	0.57
1:B:274:ASN:N	1:B:312:PRO:O	2.21	0.57
1:B:195:ARG:HE	2:B:501:C06:C	2.17	0.57
1:B:329:LYS:O	1:B:333:ALA:N	2.33	0.57
1:B:250:LYS:HZ1	2:B:501:C06:C8	2.07	0.57
1:A:41:GLU:C	1:A:45:PHE:CD2	2.74	0.57
1:A:28:ILE:HG12	1:A:69:LEU:HB2	1.87	0.57
1:B:305:LEU:HB3	1:B:309:TYR:CZ	2.40	0.57
1:A:101:PHE:HB3	1:A:118:ARG:NH2	2.20	0.56
1:A:2:PHE:CZ	1:A:6:LEU:HD13	2.39	0.56
1:A:187:ALA:HB1	2:A:501:C06:C	2.35	0.56
1:B:130:HIS:ND1	1:B:151:TYR:OH	2.39	0.56
1:B:189:ASN:CG	2:B:501:C06:C4	2.69	0.56
1:B:250:LYS:HD2	2:B:501:C06:O6	2.05	0.56
1:B:189:ASN:CB	2:B:501:C06:C1	2.76	0.56
1:B:2:PHE:CE1	1:B:5:LEU:HD23	2.41	0.56
1:B:193:PRO:HA	1:B:196:ASN:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:ND2	1:A:154:LYS:O	2.28	0.55
1:A:15:ILE:HA	1:A:329:LYS:HZ3	1.69	0.55
1:A:128:GLU:OE2	1:A:253:ASP:CG	2.44	0.55
1:A:108:ILE:HG12	1:A:120:LEU:HD23	1.89	0.55
1:B:304:TYR:O	1:B:308:LEU:HB2	2.06	0.55
1:B:190:PRO:HA	1:B:196:ASN:HD21	1.72	0.55
1:A:101:PHE:HB3	1:A:118:ARG:HH22	1.72	0.55
1:A:195:ARG:CD	2:A:501:C06:O3	2.55	0.55
1:A:229:LEU:HD22	1:A:235:ASN:ND2	2.21	0.55
1:A:128:GLU:O	1:A:132:LYS:HG2	2.07	0.54
1:B:106:TYR:HD1	1:B:118:ARG:HA	1.72	0.54
1:B:46:VAL:CB	1:B:127:ASN:OD1	2.51	0.54
1:B:49:PHE:HZ	1:B:154:LYS:NZ	2.00	0.54
1:B:6:LEU:HD22	1:B:143:TYR:HB3	1.89	0.54
1:B:88:LYS:NZ	1:B:338:ILE:O	2.31	0.54
1:A:187:ALA:CB	1:A:195:ARG:HH11	2.19	0.54
1:A:305:LEU:O	1:A:309:TYR:N	2.34	0.54
1:A:133:ALA:HA	1:A:136:VAL:HG22	1.90	0.54
1:A:316:LEU:N	1:A:319:LYS:O	2.41	0.54
1:A:229:LEU:HD22	1:A:235:ASN:HD22	1.73	0.54
1:A:334:PHE:CE2	1:A:338:ILE:HD11	2.42	0.54
1:B:128:GLU:O	1:B:132:LYS:HG2	2.08	0.53
1:A:99:PRO:HG2	1:A:119:TYR:CE2	2.43	0.53
1:A:218:LEU:HD11	1:A:228:PHE:CE1	2.44	0.53
1:A:264:TRP:HB2	1:A:281:VAL:HB	1.91	0.53
1:B:190:PRO:O	1:B:196:ASN:ND2	2.41	0.53
1:A:49:PHE:CG	1:A:130:HIS:CE1	2.97	0.53
1:B:327:SER:O	1:B:331:ILE:HD12	2.09	0.53
1:A:233:LYS:HZ3	1:A:298:HIS:CE1	2.26	0.53
1:B:195:ARG:CB	1:B:195:ARG:NH2	2.72	0.53
1:B:128:GLU:HG3	1:B:249:GLU:CB	2.39	0.53
1:B:316:LEU:HB2	1:B:321:TYR:CD2	2.44	0.53
1:A:223:LYS:O	1:B:223:LYS:HB2	2.09	0.53
1:A:72:GLY:O	1:A:104:PHE:HZ	1.92	0.53
1:A:120:LEU:HD21	1:A:331:ILE:HG23	1.91	0.53
1:A:1:MET:HG3	1:A:4:PRO:HD2	1.91	0.53
1:A:274:ASN:N	1:A:312:PRO:O	2.28	0.53
1:B:45:PHE:HA	1:B:127:ASN:ND2	2.22	0.53
1:B:247:VAL:HG21	1:B:272:ASP:OD2	2.09	0.53
1:B:5:LEU:HD13	1:B:312:PRO:HB2	1.91	0.52
1:A:122:MET:SD	1:A:331:ILE:HD13	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ASP:HB3	1:B:113:LEU:HD13	1.91	0.52
1:B:225:LYS:HZ1	2:B:501:C06:C9	2.11	0.52
1:A:108:ILE:HA	1:A:120:LEU:O	2.10	0.52
1:A:85:GLN:CB	1:A:349:PRO:HG3	2.39	0.52
1:B:266:SER:HB3	1:B:269:VAL:HB	1.91	0.52
1:A:195:ARG:NE	2:A:501:C06:C	2.70	0.52
1:B:3:GLN:OE1	1:B:6:LEU:CD2	2.58	0.51
2:A:501:C06:O9	1:B:223:LYS:HB3	2.10	0.51
1:B:250:LYS:CD	2:B:501:C06:O4	2.54	0.51
1:B:138:ASP:OD1	1:B:139:THR:N	2.44	0.51
1:B:277:SER:HA	1:B:307:MET:HG3	1.92	0.51
1:B:195:ARG:CB	1:B:195:ARG:HH21	2.24	0.51
1:A:164:HIS:HB3	1:A:167:LEU:HB3	1.91	0.51
1:A:48:TYR:CE2	1:A:57:ILE:HG21	2.45	0.51
1:B:183:ALA:HB3	1:B:208:VAL:HG22	1.93	0.51
1:B:27:LYS:HG3	1:B:58:THR:HB	1.93	0.51
1:A:127:ASN:O	1:A:131:ILE:CD1	2.58	0.51
1:B:297:LEU:HD23	1:B:303:ALA:HB1	1.92	0.51
1:A:187:ALA:CB	1:A:195:ARG:NH1	2.69	0.50
1:A:210:GLY:HA3	1:A:215:ARG:O	2.11	0.50
1:A:260:ILE:HD12	1:A:304:TYR:CE1	2.47	0.50
1:A:237:CYS:SG	1:A:261:PRO:HB3	2.52	0.50
1:B:34:TRP:HB3	1:B:38:GLU:HB2	1.93	0.50
1:A:202:LEU:HA	1:A:291:ILE:HD12	1.94	0.50
1:B:119:TYR:HE2	1:B:121:ARG:HB2	1.75	0.50
1:B:22:SER:O	1:B:22:SER:OG	2.24	0.49
1:A:42:PHE:HD1	1:A:45:PHE:HZ	1.59	0.49
1:B:106:TYR:CE2	1:B:338:ILE:HG12	2.47	0.49
1:A:31:ALA:HB2	1:A:72:GLY:HA3	1.93	0.49
1:A:253:ASP:O	1:A:257:SER:OG	2.27	0.49
1:B:194:ILE:HG22	1:B:238:PHE:HD2	1.76	0.49
1:A:178:LEU:HD23	1:A:233:LYS:NZ	2.28	0.48
1:A:240:ASN:CA	2:A:501:C06:O13	2.60	0.48
1:B:2:PHE:HB3	1:B:143:TYR:CE1	2.48	0.48
1:B:1:MET:N	1:B:308:LEU:O	2.40	0.48
1:A:128:GLU:OE2	1:A:253:ASP:OD2	2.30	0.48
1:A:297:LEU:O	1:A:304:TYR:HB2	2.13	0.48
1:A:42:PHE:N	1:A:45:PHE:CE2	2.81	0.48
1:A:115:PHE:HB3	1:A:118:ARG:HB2	1.95	0.48
1:A:23:PRO:O	1:A:56:THR:OG1	2.26	0.48
1:A:240:ASN:OD1	1:A:240:ASN:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:VAL:HG12	1:A:215:ARG:HG2	1.95	0.48
1:B:240:ASN:N	1:B:240:ASN:OD1	2.47	0.48
1:B:109:GLY:O	1:B:122:MET:N	2.37	0.48
1:B:23:PRO:HB2	1:B:56:THR:OG1	2.13	0.48
1:A:111:ASP:HB3	1:A:113:LEU:HB2	1.95	0.48
1:B:203:ASN:C	1:B:205:ILE:H	2.18	0.48
1:B:316:LEU:HB2	1:B:321:TYR:HD2	1.79	0.48
1:A:167:LEU:HD13	1:A:257:SER:HA	1.95	0.47
1:A:138:ASP:OD1	1:A:139:THR:N	2.47	0.47
1:B:105:ASP:O	1:B:118:ARG:NH2	2.46	0.47
1:B:149:SER:O	1:B:153:LEU:HG	2.13	0.47
1:B:138:ASP:OD2	1:B:159:CYS:N	2.39	0.47
1:B:138:ASP:HB3	1:B:141:ALA:HB2	1.97	0.47
1:B:266:SER:O	1:B:269:VAL:HG12	2.14	0.47
1:A:190:PRO:O	1:A:192:ALA:N	2.47	0.47
1:A:21:LYS:O	1:A:23:PRO:HD3	2.14	0.47
1:B:330:LYS:O	1:B:334:PHE:HB2	2.15	0.47
1:A:239:GLU:OE1	1:A:248:THR:OG1	2.28	0.47
1:A:38:GLU:HG3	1:B:218:LEU:HD23	1.96	0.47
1:B:185:PHE:N	1:B:209:THR:O	2.48	0.47
1:A:142:PRO:HB3	1:A:172:ASN:OD1	2.14	0.46
1:B:29:ALA:HB3	1:B:70:VAL:HG13	1.97	0.46
1:A:41:GLU:C	1:A:45:PHE:CE2	2.89	0.46
1:B:183:ALA:HA	1:B:234:PHE:HB2	1.97	0.46
1:A:220:TYR:OH	1:B:37:GLU:HG2	2.15	0.46
1:A:266:SER:C	1:A:268:SER:H	2.19	0.46
1:A:29:ALA:N	1:A:69:LEU:O	2.43	0.46
1:B:195:ARG:CZ	1:B:195:ARG:HB2	2.46	0.46
1:B:25:PRO:HA	1:B:56:THR:HB	1.98	0.46
1:A:279:VAL:HG13	1:A:293:TYR:HD2	1.81	0.46
1:B:195:ARG:CD	2:B:501:C06:P	2.97	0.46
1:A:72:GLY:O	1:A:104:PHE:CZ	2.68	0.46
1:B:139:THR:HG23	1:B:156:PRO:HB2	1.98	0.46
1:B:195:ARG:NE	2:B:501:C06:C1	2.58	0.46
1:B:192:ALA:HB2	2:B:501:C06:O13	2.15	0.46
1:A:246:TYR:O	1:A:263:TYR:OH	2.34	0.46
1:A:263:TYR:N	1:A:279:VAL:O	2.46	0.46
1:A:111:ASP:HB2	1:A:119:TYR:OH	2.15	0.46
1:A:187:ALA:CA	1:A:195:ARG:HH11	2.29	0.46
1:A:149:SER:OG	1:A:150:LEU:N	2.49	0.45
1:B:3:GLN:O	1:B:7:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ILE:O	1:B:256:PHE:N	2.46	0.45
1:A:42:PHE:N	1:A:45:PHE:HE2	2.15	0.45
1:B:128:GLU:OE1	1:B:132:LYS:HE2	2.17	0.45
1:B:238:PHE:CZ	1:B:281:VAL:HG21	2.52	0.45
1:A:96:ASN:HA	1:A:110:PHE:CZ	2.52	0.45
1:A:194:ILE:HG21	1:A:264:TRP:CD2	2.51	0.45
1:A:233:LYS:NZ	1:A:298:HIS:CE1	2.85	0.45
1:A:45:PHE:HE1	1:A:92:TYR:HE2	1.61	0.45
1:A:203:ASN:OD1	1:A:208:VAL:N	2.49	0.45
1:B:121:ARG:HB3	1:B:324:GLN:OE1	2.17	0.45
1:A:85:GLN:HB2	1:A:349:PRO:HG3	1.99	0.44
1:B:51:LEU:C	1:B:53:GLN:H	2.18	0.44
1:A:262:ILE:HG23	1:A:279:VAL:HG11	1.99	0.44
1:B:185:PHE:O	1:B:210:GLY:HA2	2.17	0.44
1:B:23:PRO:HA	1:B:24:PRO:HD2	1.88	0.44
1:A:166:ASN:OD1	1:A:230:SER:OG	2.31	0.44
1:A:248:THR:HG1	1:A:250:LYS:NZ	2.09	0.44
1:B:51:LEU:O	1:B:54:ARG:N	2.45	0.44
1:A:128:GLU:HB2	1:A:249:GLU:HB2	1.98	0.44
1:A:1:MET:N	1:A:312:PRO:HD3	2.32	0.44
1:B:186:VAL:HG21	1:B:229:LEU:HD21	1.99	0.44
1:B:194:ILE:HG22	1:B:238:PHE:CE2	2.53	0.44
1:B:108:ILE:HG23	1:B:120:LEU:HD23	2.00	0.44
1:B:164:HIS:HB3	1:B:167:LEU:HB3	2.00	0.44
1:B:183:ALA:HB3	1:B:208:VAL:HG13	1.99	0.44
1:A:42:PHE:HE2	1:A:59:LEU:HD22	1.81	0.44
1:B:343:THR:HB	1:B:345:TYR:CZ	2.53	0.44
1:A:238:PHE:O	2:A:501:C06:P	2.76	0.44
1:A:22:SER:O	1:A:22:SER:OG	2.25	0.44
1:A:233:LYS:NZ	1:A:298:HIS:ND1	2.65	0.44
1:A:85:GLN:HB3	1:A:349:PRO:HG3	2.00	0.44
1:B:337:THR:HA	1:B:340:ASP:HB2	2.00	0.44
1:A:185:PHE:O	1:A:211:GLY:N	2.51	0.43
1:A:71:PHE:HB3	1:A:72:GLY:H	1.73	0.43
1:A:21:LYS:C	1:A:23:PRO:HD3	2.38	0.43
1:A:199:ASN:O	1:A:203:ASN:HB2	2.18	0.43
1:B:42:PHE:CB	1:B:45:PHE:HE2	2.30	0.43
1:A:293:TYR:O	1:A:297:LEU:HG	2.18	0.43
1:B:106:TYR:CD1	1:B:118:ARG:HA	2.53	0.43
1:A:225:LYS:CD	2:A:501:C06:O10	2.38	0.43
1:A:195:ARG:HG3	1:A:195:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:HG21	1:B:232:TYR:OH	2.19	0.43
1:B:51:LEU:C	1:B:53:GLN:N	2.72	0.43
1:A:241:THR:HG1	1:A:246:TYR:HE2	1.67	0.43
1:A:245:GLY:O	1:A:247:VAL:N	2.49	0.43
1:A:233:LYS:HZ3	1:A:298:HIS:CG	2.37	0.43
1:A:348:ASN:HB3	1:A:350:PHE:CZ	2.54	0.43
1:A:41:GLU:HG2	1:A:45:PHE:CD2	2.54	0.43
1:A:280:ASN:HB3	1:A:283:ASP:OD2	2.18	0.43
1:A:306:ASP:O	1:A:310:GLU:HG2	2.19	0.43
1:B:301:LYS:O	1:B:305:LEU:HG	2.19	0.43
1:A:235:ASN:O	1:A:262:ILE:N	2.45	0.43
1:B:195:ARG:HD3	2:B:501:C06:P	2.59	0.43
1:A:138:ASP:OD1	1:A:158:HIS:HA	2.19	0.42
1:B:111:ASP:N	1:B:119:TYR:HH	2.16	0.42
1:B:190:PRO:O	1:B:192:ALA:N	2.50	0.42
1:B:42:PHE:CE1	1:B:45:PHE:CZ	2.84	0.42
1:B:27:LYS:HB3	1:B:60:HIS:CE1	2.55	0.42
1:A:96:ASN:HA	1:A:110:PHE:CE1	2.54	0.42
1:B:125:TYR:HB3	1:B:248:THR:O	2.19	0.42
1:B:296:TYR:HE1	1:B:303:ALA:HB2	1.83	0.42
1:A:121:ARG:CZ	1:A:123:PRO:HG3	2.50	0.42
1:A:334:PHE:O	1:A:338:ILE:HG13	2.19	0.42
1:B:48:TYR:CD1	1:B:57:ILE:HD13	2.54	0.42
1:B:183:ALA:CB	1:B:208:VAL:HG13	2.49	0.42
1:B:180:ARG:HB2	1:B:233:LYS:CG	2.48	0.42
1:B:250:LYS:HD2	2:B:501:C06:O7	2.19	0.42
1:B:316:LEU:N	1:B:319:LYS:O	2.41	0.42
1:A:255:TYR:CE2	1:A:312:PRO:HB3	2.55	0.42
1:A:26:LEU:HD23	1:A:57:ILE:HG12	2.00	0.42
1:B:69:LEU:CD2	1:B:338:ILE:HG21	2.49	0.42
1:A:109:GLY:O	1:A:122:MET:N	2.52	0.42
1:A:165:PRO:HD2	1:A:227:GLU:CD	2.40	0.42
1:A:177:PRO:O	1:A:233:LYS:HG2	2.19	0.42
1:A:108:ILE:HG23	1:A:122:MET:HB2	2.02	0.42
1:A:218:LEU:HD11	1:A:228:PHE:HE1	1.84	0.42
1:B:185:PHE:CE2	1:B:215:ARG:HB2	2.55	0.42
1:B:285:LYS:HB3	1:B:285:LYS:HE3	1.63	0.42
1:A:51:LEU:HD13	1:A:57:ILE:HD11	2.01	0.41
1:A:59:LEU:O	1:A:60:HIS:HD2	2.03	0.41
1:A:37:GLU:OE2	1:B:231:GLN:CD	2.58	0.41
1:B:34:TRP:HB3	1:B:35:GLY:H	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:GLN:HG3	1:B:3:GLN:O	2.20	0.41
1:A:165:PRO:HD2	1:A:227:GLU:OE1	2.20	0.41
1:A:2:PHE:HD2	1:A:143:TYR:CD1	2.37	0.41
1:B:250:LYS:NZ	2:B:501:C06:C8	2.74	0.41
1:A:49:PHE:O	1:A:52:SER:OG	2.30	0.41
1:B:140:THR:O	1:B:160:PHE:HB3	2.20	0.41
1:B:185:PHE:CZ	1:B:187:ALA:HB3	2.56	0.41
1:B:41:GLU:C	1:B:45:PHE:CD2	2.94	0.41
1:B:101:PHE:HB3	1:B:118:ARG:NH2	2.35	0.41
1:B:189:ASN:CA	2:B:501:C06:C2	2.97	0.41
1:A:42:PHE:CD1	1:A:45:PHE:HZ	2.37	0.41
1:B:195:ARG:HD3	2:B:501:C06:O	2.21	0.41
1:B:138:ASP:OD2	1:B:160:PHE:N	2.53	0.41
1:B:26:LEU:HD11	1:B:69:LEU:HD12	2.03	0.41
1:A:335:PHE:CD1	1:A:338:ILE:HD12	2.55	0.41
1:B:85:GLN:HG2	1:B:85:GLN:H	1.69	0.41
1:A:99:PRO:CG	1:A:119:TYR:HE2	2.32	0.41
1:A:250:LYS:HD3	2:A:501:C06:O4	2.21	0.40
1:B:118:ARG:HE	1:B:118:ARG:HB3	1.78	0.40
1:B:248:THR:HB	1:B:249:GLU:H	1.79	0.40
1:B:296:TYR:HA	1:B:300:HIS:ND1	2.36	0.40
1:B:264:TRP:CD1	1:B:281:VAL:HB	2.48	0.40
1:A:229:LEU:HG	1:A:229:LEU:H	1.70	0.40
1:A:327:SER:O	1:A:331:ILE:HG13	2.22	0.40
1:A:150:LEU:HD23	1:A:328:PHE:HE2	1.86	0.40
1:A:42:PHE:HE2	1:A:59:LEU:CD2	2.35	0.40
1:A:73:ASN:HA	1:A:74:PRO:HD2	1.74	0.40
1:B:239:GLU:HA	2:B:501:C06:O2	2.21	0.40
1:A:96:ASN:OD1	1:A:110:PHE:HZ	2.05	0.40
1:B:101:PHE:HB3	1:B:118:ARG:HH22	1.87	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LYS:NZ	1:B:345:TYR:OH[2_445]	1.79	0.41

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	339/420 (81%)	282 (83%)	48 (14%)	9 (3%)	5	30
1	B	339/420 (81%)	278 (82%)	58 (17%)	3 (1%)	17	56
All	All	678/840 (81%)	560 (83%)	106 (16%)	12 (2%)	8	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	B	182	PHE
1	A	340	ASP
1	A	283	ASP
1	A	142	PRO
1	A	246	TYR
1	B	52	SER
1	A	191	ASN
1	A	218	LEU
1	A	92	TYR
1	B	190	PRO
1	A	22	SER

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	308/382 (81%)	294 (96%)	14 (4%)	27	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	308/382 (81%)	294 (96%)	14 (4%)	27	63
All	All	616/764 (81%)	588 (96%)	28 (4%)	27	63

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	22	SER
1	A	27	LYS
1	A	105	ASP
1	A	115	PHE
1	A	126	TYR
1	A	147	ASP
1	A	176	ASP
1	A	205	ILE
1	A	246	TYR
1	A	266	SER
1	A	287	PHE
1	A	298	HIS
1	A	301	LYS
1	B	3	GLN
1	B	18	MET
1	B	27	LYS
1	B	36	ASP
1	B	58	THR
1	B	84	TYR
1	B	92	TYR
1	B	115	PHE
1	B	195	ARG
1	B	221	ASN
1	B	255	TYR
1	B	288	ASP
1	B	319	LYS
1	B	340	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	B	196	ASN
1	B	231	GLN

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Mol	Chain	Res	Type
1	B	258	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
2	C06	B	501	-	34,41,41	1.49	6 (17%)	46,64,64	2.10	10 (21%)
2	C06	A	501	-	34,41,41	1.50	7 (20%)	46,64,64	2.10	10 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C06	B	501	-	-	2/17/57/57	0/4/4/4
2	C06	A	501	-	-	2/17/57/57	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	C06	C15-C12	4.09	1.48	1.41
2	B	501	C06	C15-C12	4.06	1.48	1.41
2	B	501	C06	C14-N4	3.87	1.41	1.33
2	A	501	C06	C14-N4	3.85	1.41	1.33
2	A	501	C06	P-O3	2.96	1.61	1.50
2	B	501	C06	C15-N3	2.96	1.38	1.33
2	B	501	C06	P-O3	2.96	1.61	1.50
2	A	501	C06	C15-N3	2.93	1.38	1.33
2	A	501	C06	C14-N3	2.34	1.39	1.35
2	B	501	C06	C14-N3	2.33	1.39	1.35
2	A	501	C06	C12-C13	2.10	1.46	1.40
2	B	501	C06	C12-C13	2.08	1.46	1.40
2	A	501	C06	O8-C10	2.02	1.43	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	C06	C14-N2-C13	8.04	124.54	115.36
2	B	501	C06	C14-N2-C13	8.01	124.51	115.36
2	A	501	C06	N2-C14-N3	-5.95	119.28	127.22
2	B	501	C06	N2-C14-N3	-5.93	119.31	127.22
2	A	501	C06	C15-N3-C14	3.60	121.66	115.93
2	B	501	C06	C15-N3-C14	3.58	121.62	115.93
2	A	501	C06	P1-O4-P	-3.58	120.54	132.83
2	B	501	C06	P1-O4-P	-3.58	120.55	132.83
2	A	501	C06	N4-C14-N3	3.57	122.81	117.25
2	B	501	C06	N4-C14-N3	3.57	122.80	117.25
2	B	501	C06	C12-C15-N3	-3.50	118.65	123.43
2	A	501	C06	C12-C15-N3	-3.48	118.67	123.43
2	A	501	C06	C15-C12-C13	-3.09	117.84	120.80
2	B	501	C06	O4-P-O1	3.08	108.69	102.48
2	A	501	C06	O4-P-O1	3.07	108.67	102.48
2	B	501	C06	C15-C12-C13	-3.05	117.88	120.80
2	A	501	C06	C13-C12-N1	-2.89	106.38	109.40
2	B	501	C06	C13-C12-N1	-2.89	106.38	109.40
2	B	501	C06	O-C5-O1	-2.06	108.68	111.36
2	A	501	C06	O-C5-O1	-2.03	108.71	111.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

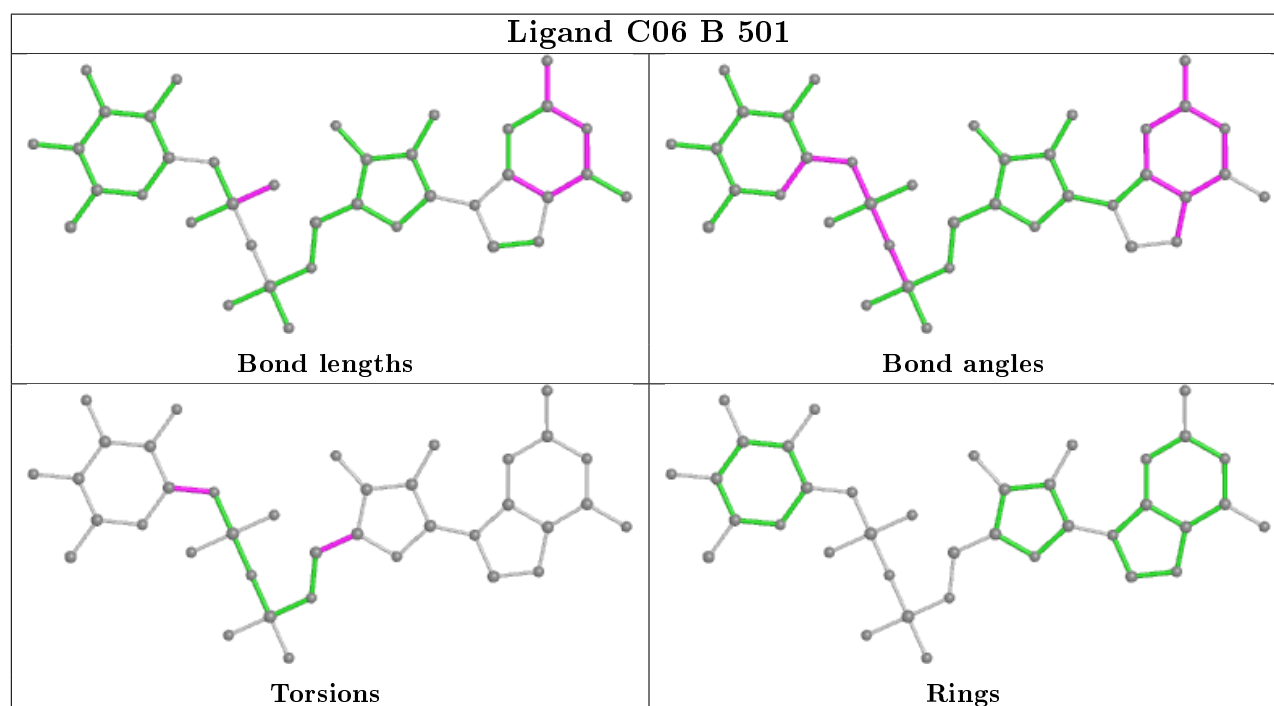
Mol	Chain	Res	Type	Atoms
2	B	501	C06	C4-C5-O1-P
2	A	501	C06	C4-C5-O1-P
2	B	501	C06	O7-C6-C7-O8
2	A	501	C06	O7-C6-C7-O8

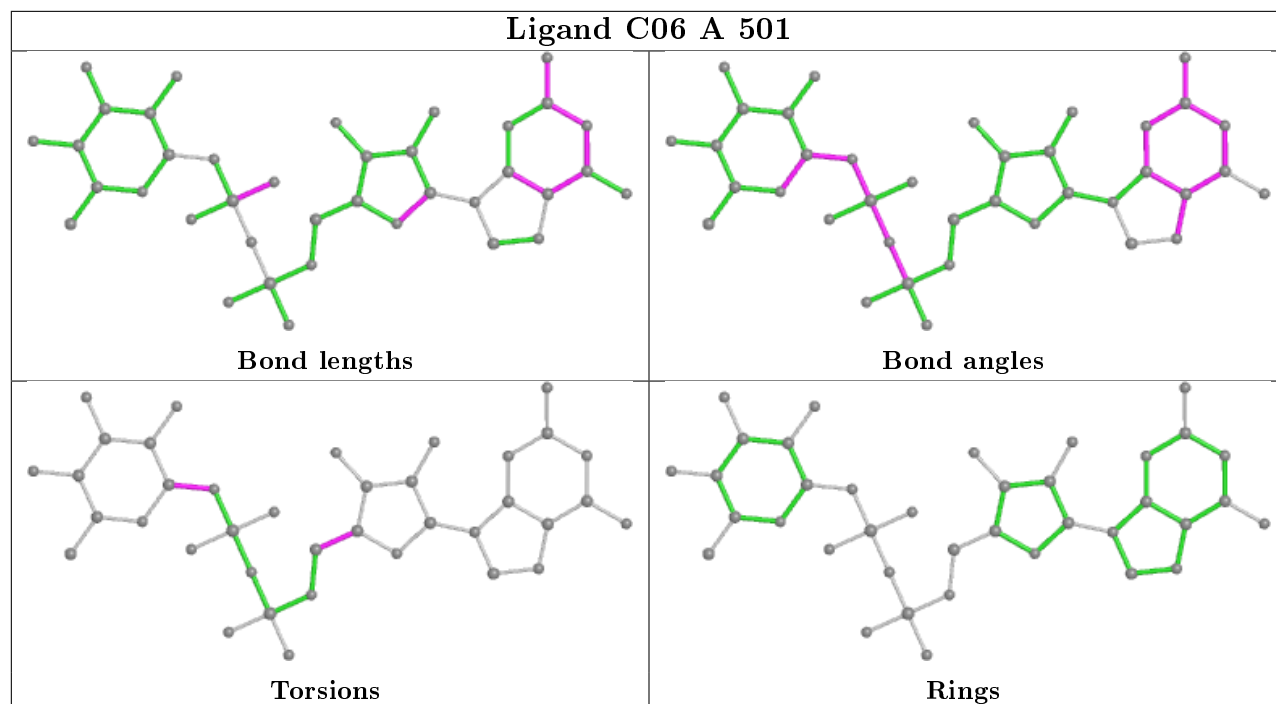
There are no ring outliers.

2 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	C06	56	0
2	A	501	C06	33	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	343/420 (81%)	1.87	130 (37%) 0 0	11, 33, 52, 96	0
1	B	343/420 (81%)	1.93	131 (38%) 0 0	12, 29, 60, 80	0
All	All	686/840 (81%)	1.90	261 (38%) 0 0	11, 32, 56, 96	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	GLY	13.4
1	A	259	THR	9.4
1	B	287	PHE	8.1
1	A	18	MET	7.5
1	B	34	TRP	7.3
1	A	91	PHE	7.3
1	B	108	ILE	7.0
1	B	203	ASN	6.9
1	B	327	SER	6.8
1	B	260	ILE	6.8
1	B	303	ALA	6.8
1	B	30	VAL	6.8
1	B	351	ILE	6.6
1	A	20	SER	6.5
1	B	188	SER	6.4
1	A	228	PHE	6.3
1	B	57	ILE	6.2
1	B	304	TYR	6.1
1	B	61	GLN	6.0
1	B	320	ALA	5.8
1	B	19	ALA	5.5
1	B	35	GLY	5.4
1	B	347	ASP	5.3
1	A	88	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	204	SER	5.3
1	A	58	THR	5.2
1	B	1	MET	5.1
1	A	112	GLU	4.9
1	B	116	ASN	4.8
1	A	57	ILE	4.8
1	A	21	LYS	4.8
1	A	284	PHE	4.7
1	A	120	LEU	4.7
1	A	257	SER	4.7
1	A	94	GLY	4.7
1	A	159	CYS	4.6
1	B	136	VAL	4.6
1	A	86	ASN	4.6
1	B	259	THR	4.6
1	B	8	ALA	4.6
1	A	73	ASN	4.5
1	B	32	ASN	4.5
1	B	9	TYR	4.4
1	B	29	ALA	4.3
1	B	31	ALA	4.3
1	B	14	SER	4.3
1	B	67	SER	4.3
1	B	98	SER	4.2
1	B	91	PHE	4.2
1	A	107	ALA	4.2
1	B	96	ASN	4.2
1	B	18	MET	4.1
1	B	58	THR	4.1
1	A	194	ILE	4.1
1	A	141	ALA	4.0
1	A	299	THR	4.0
1	A	317	ASP	4.0
1	A	108	ILE	4.0
1	A	184	SER	4.0
1	B	232	TYR	3.9
1	A	316	LEU	3.9
1	A	87	ALA	3.9
1	A	260	ILE	3.9
1	B	257	SER	3.9
1	A	29	ALA	3.9
1	A	30	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	93	THR	3.9
1	B	107	ALA	3.8
1	A	255	TYR	3.8
1	B	50	ILE	3.8
1	B	56	THR	3.8
1	A	318	GLY	3.8
1	A	19	ALA	3.7
1	A	4	PRO	3.7
1	A	56	THR	3.7
1	A	25	PRO	3.7
1	B	288	ASP	3.7
1	A	352	PHE	3.7
1	A	193	PRO	3.7
1	A	36	ASP	3.7
1	B	321	TYR	3.7
1	B	93	THR	3.6
1	A	168	CYS	3.6
1	B	247	VAL	3.6
1	A	1	MET	3.6
1	A	216	ASN	3.6
1	B	213	SER	3.6
1	A	283	ASP	3.6
1	B	324	GLN	3.5
1	A	142	PRO	3.5
1	A	24	PRO	3.5
1	A	236	LEU	3.5
1	A	156	PRO	3.5
1	A	181	GLY	3.5
1	B	5	LEU	3.4
1	B	164	HIS	3.4
1	A	258	HIS	3.4
1	A	153	LEU	3.4
1	B	286	ASN	3.4
1	B	54	ARG	3.4
1	A	63	PRO	3.3
1	B	335	PHE	3.3
1	B	265	GLY	3.3
1	A	346	HIS	3.3
1	B	41	GLU	3.3
1	A	92	TYR	3.3
1	B	70	VAL	3.2
1	B	100	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	99	PRO	3.2
1	A	64	ASN	3.2
1	B	125	TYR	3.2
1	A	191	ASN	3.2
1	A	40	LYS	3.1
1	B	168	CYS	3.1
1	B	65	GLU	3.1
1	B	224	ASN	3.1
1	A	178	LEU	3.1
1	A	217	THR	3.1
1	B	155	LYS	3.1
1	B	60	HIS	3.1
1	B	68	ASP	3.1
1	B	323	TYR	3.1
1	B	187	ALA	3.1
1	A	263	TYR	3.0
1	A	115	PHE	3.0
1	B	25	PRO	3.0
1	B	316	LEU	3.0
1	A	54	ARG	3.0
1	B	174	GLU	3.0
1	B	240	ASN	3.0
1	A	16	GLU	3.0
1	A	155	LYS	3.0
1	B	254	ALA	3.0
1	A	50	ILE	3.0
1	A	351	ILE	3.0
1	A	134	GLU	3.0
1	B	138	ASP	2.9
1	A	224	ASN	2.9
1	B	112	GLU	2.9
1	A	66	PHE	2.9
1	A	324	GLN	2.9
1	A	285	LYS	2.9
1	A	270	ALA	2.9
1	A	247	VAL	2.9
1	B	284	PHE	2.9
1	A	277	SER	2.8
1	B	36	ASP	2.8
1	A	65	GLU	2.8
1	B	201	ALA	2.8
1	A	226	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	20	SER	2.8
1	A	100	ASN	2.8
1	B	113	LEU	2.8
1	B	212	GLY	2.8
1	A	28	ILE	2.8
1	B	66	PHE	2.8
1	B	237	CYS	2.8
1	A	61	GLN	2.7
1	A	234	PHE	2.7
1	B	92	TYR	2.7
1	A	160	PHE	2.7
1	B	246	TYR	2.7
1	A	137	ASN	2.7
1	A	167	LEU	2.7
1	A	213	SER	2.7
1	B	149	SER	2.7
1	A	157	SER	2.7
1	B	135	SER	2.7
1	A	147	ASP	2.7
1	B	86	ASN	2.7
1	A	5	LEU	2.7
1	A	225	LYS	2.7
1	A	126	TYR	2.6
1	A	268	SER	2.6
1	B	348	ASN	2.6
1	B	7	ASP	2.6
1	A	6	LEU	2.6
1	B	15	ILE	2.6
1	B	339	LEU	2.6
1	A	261	PRO	2.6
1	B	28	ILE	2.6
1	A	114	ASP	2.6
1	B	350	PHE	2.6
1	A	101	PHE	2.6
1	B	255	TYR	2.6
1	B	38	GLU	2.5
1	A	35	GLY	2.5
1	A	133	ALA	2.5
1	B	233	LYS	2.5
1	B	280	ASN	2.5
1	B	249	GLU	2.5
1	A	304	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	48	TYR	2.5
1	B	126	TYR	2.5
1	A	70	VAL	2.5
1	A	139	THR	2.5
1	A	301	LYS	2.5
1	B	163	LYS	2.5
1	A	296	TYR	2.4
1	A	345	TYR	2.4
1	A	138	ASP	2.4
1	A	315	THR	2.4
1	A	291	ILE	2.4
1	A	158	HIS	2.4
1	B	124	LEU	2.4
1	B	202	LEU	2.4
1	B	268	SER	2.4
1	B	23	PRO	2.4
1	B	267	PRO	2.4
1	B	315	THR	2.4
1	A	237	CYS	2.4
1	A	161	LYS	2.4
1	B	158	HIS	2.4
1	B	319	LYS	2.4
1	B	242	GLN	2.4
1	B	27	LYS	2.4
1	B	190	PRO	2.3
1	B	139	THR	2.3
1	B	352	PHE	2.3
1	B	2	PHE	2.3
1	A	121	ARG	2.3
1	A	183	ALA	2.3
1	A	116	ASN	2.3
1	B	189	ASN	2.3
1	B	103	LEU	2.3
1	A	182	PHE	2.3
1	B	175	SER	2.2
1	B	243	GLY	2.2
1	A	233	LYS	2.2
1	B	102	ASN	2.2
1	B	63	PRO	2.2
1	B	143	TYR	2.2
1	A	27	LYS	2.2
1	A	146	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	165	PRO	2.2
1	A	55	TYR	2.1
1	B	140	THR	2.1
1	B	205	ILE	2.1
1	B	132	LYS	2.1
1	A	300	HIS	2.1
1	A	212	GLY	2.1
1	B	228	PHE	2.1
1	B	227	GLU	2.1
1	B	122	MET	2.1
1	A	327	SER	2.1
1	A	48	TYR	2.1
1	A	102	ASN	2.1
1	A	41	GLU	2.1
1	B	184	SER	2.1
1	B	253	ASP	2.1
1	A	338	ILE	2.1
1	B	88	LYS	2.0
1	B	289	GLU	2.0
1	A	52	SER	2.0
1	A	44	ASN	2.0
1	A	337	THR	2.0
1	B	238	PHE	2.0
1	A	69	LEU	2.0
1	A	314	ASN	2.0
1	A	53	GLN	2.0
1	B	129	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 carbohydrates in this entry.

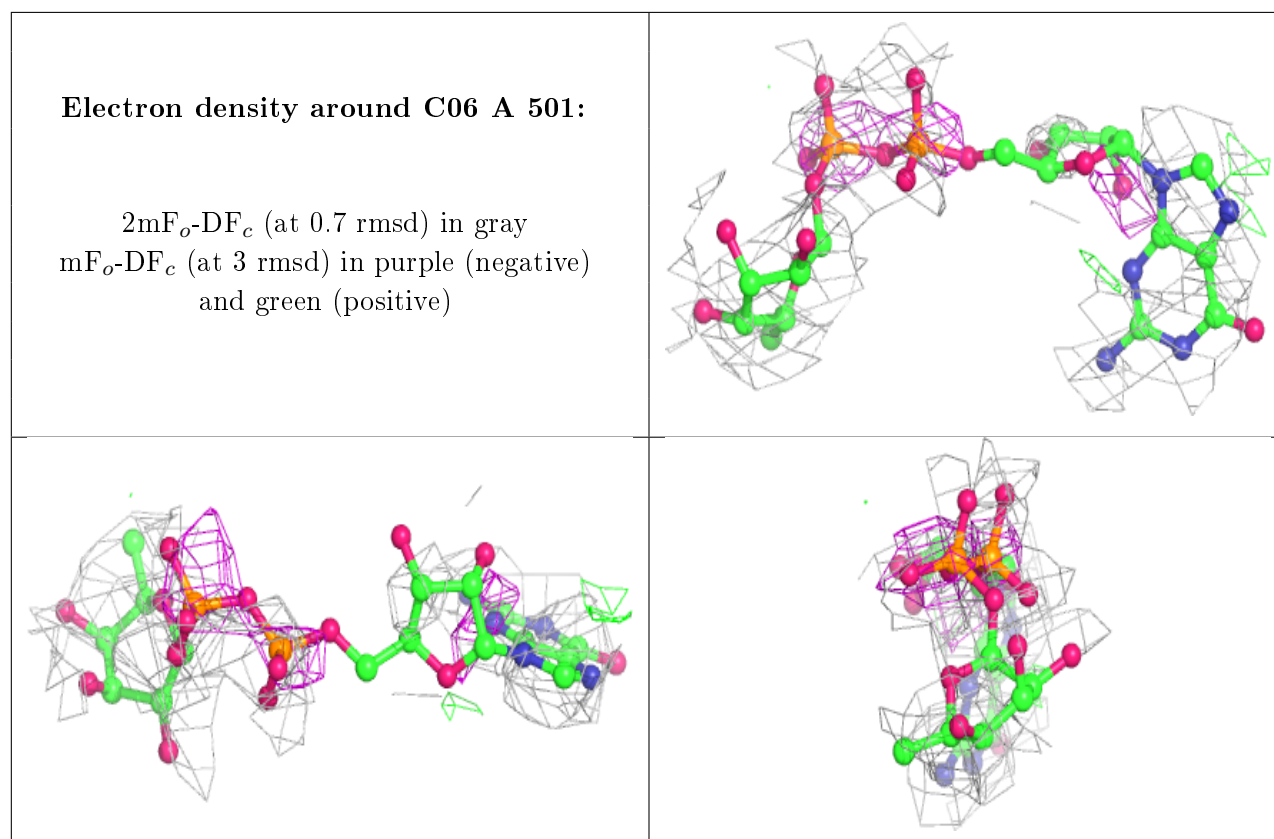
6.4 Ligands [i](#)

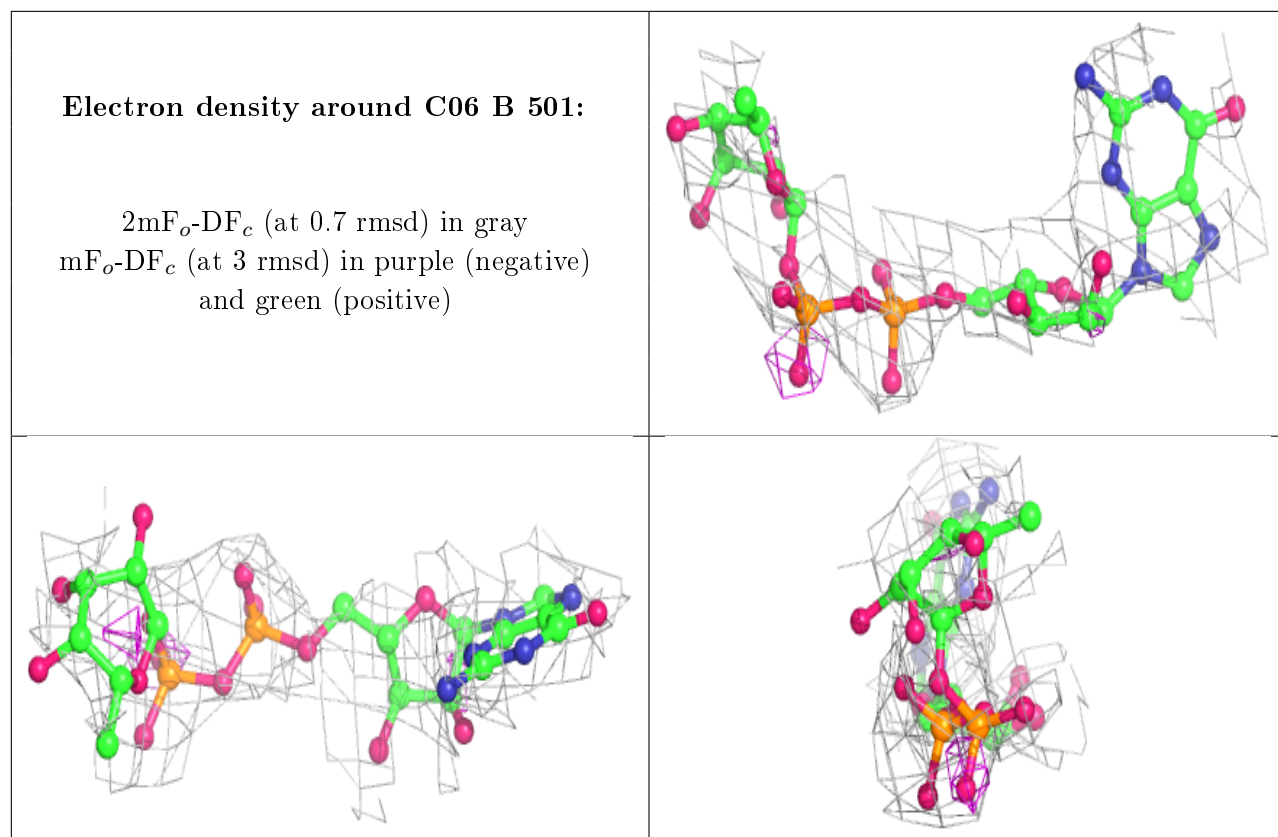
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
2	C06	A	501	38/38	0.43	0.64	20,20,20,20	0
2	C06	B	501	38/38	0.60	0.48	20,20,20,20	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.