Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2026 – 06:17 PM JST

PDB ID	:	9UIZ / pdb_00009uiz
Title	:	PLASMODIUM VIVAX PHENYLALANYL-TRNA SYNTHETASE IN COMPLEX WITH PHE-AMS IN SPACE GROUP P21
Authors	:	Mutharasappan, N.; Manickam, Y.; Bagale, S.; Pradeepkumar, P.I.; Sharma, A.
Deposited on	:	2025-04-16
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

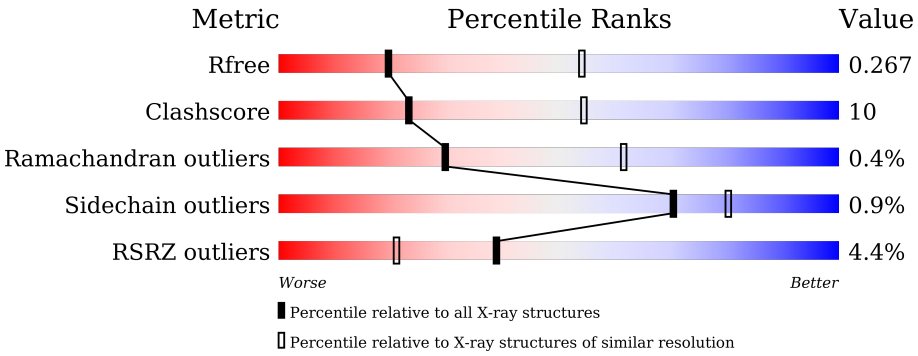
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

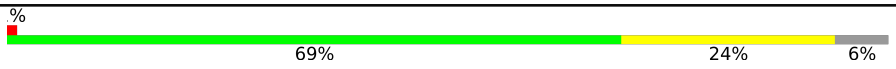
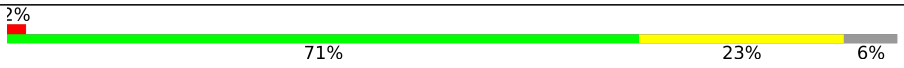
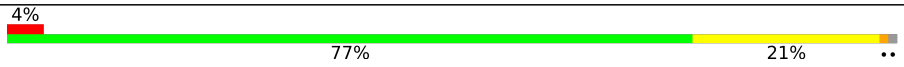
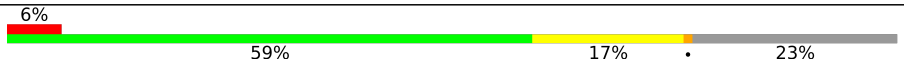
The reported resolution of this entry is 3.10 Å.

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	299	
1	C	299	
2	B	618	
2	D	618	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12760 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 Phenylalanyl-tRNA synthetase beta chain, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2298	1484	387	416	11			
1	C	282	Total	C	N	O	S	0	0	0
			2286	1478	381	416	11			

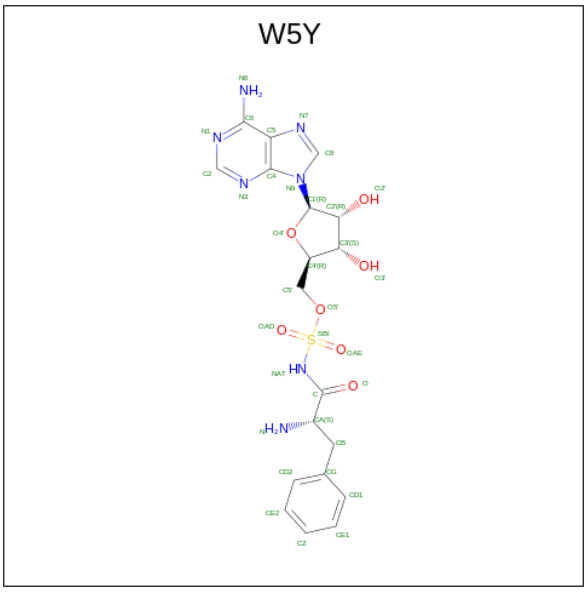
- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	612	Total	C	N	O	S	0	0	0
			4537	2880	755	878	24			
2	D	475	Total	C	N	O	S	0	0	0
			3559	2267	592	679	21			

There are 4 discrepancies between the modelled and reference sequences:

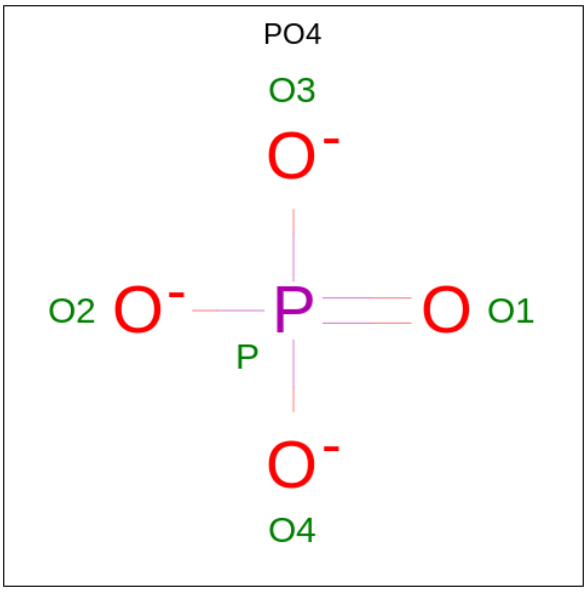
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP A5K464
B	1	GLY	-	expression tag	UNP A5K464
D	0	MET	-	expression tag	UNP A5K464
D	1	GLY	-	expression tag	UNP A5K464

- Molecule 3 is 5'-O-(L-phenylalanylsulfamoyl)adenosine (CCD ID: W5Y) (formula: $C_{19}H_{23}N_7O_7S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			34	19	7	7	1		
3	C	1	Total	C	N	O	S	0	0
			34	19	7	7	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O P 5 4 1	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

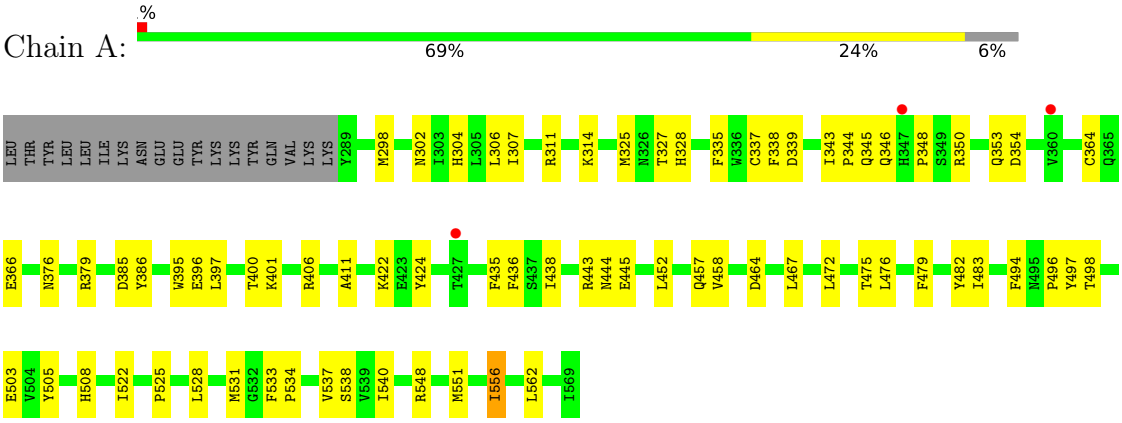
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

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.

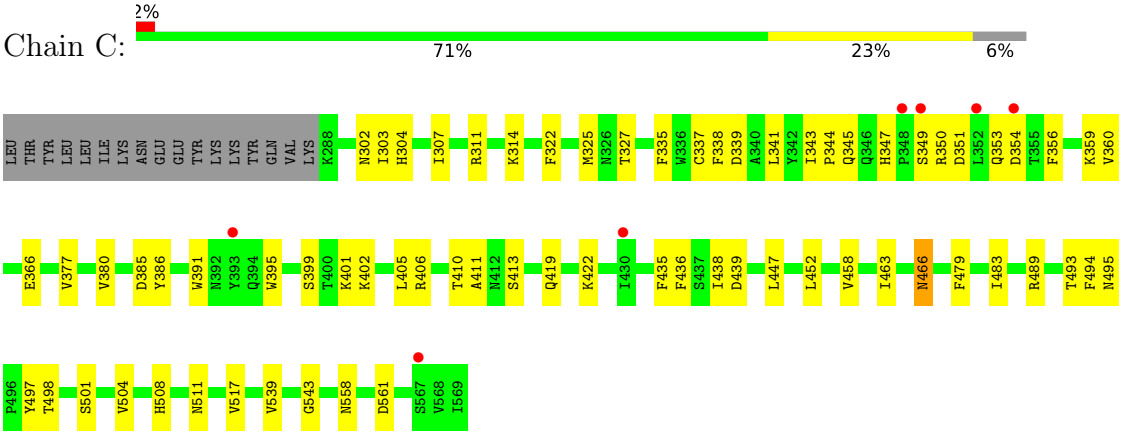
• Molecule 1: Phenylalanyl-tRNA synthetase beta chain, putative

Chain A:



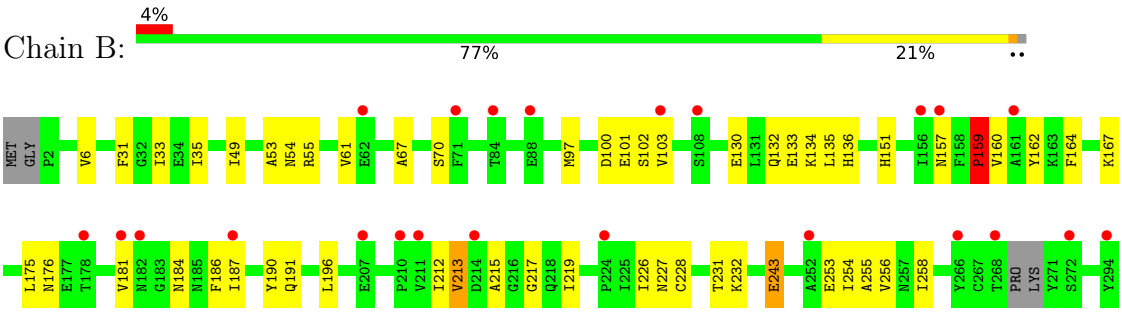
• Molecule 1: Phenylalanyl-tRNA synthetase beta chain, putative

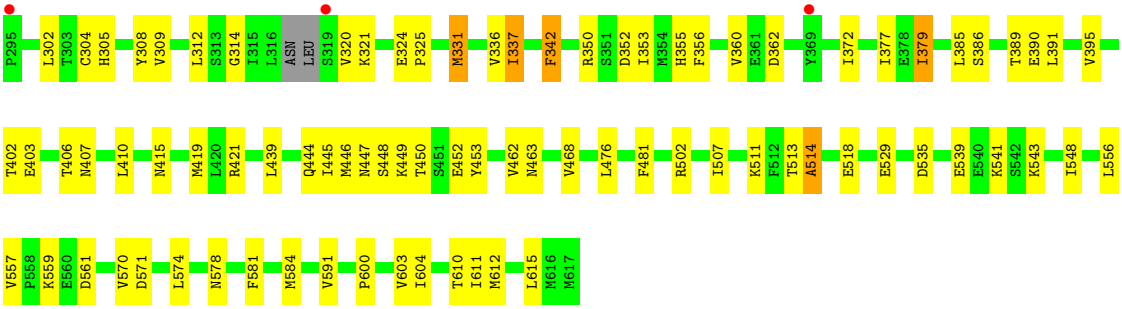
Chain C:



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain, putative

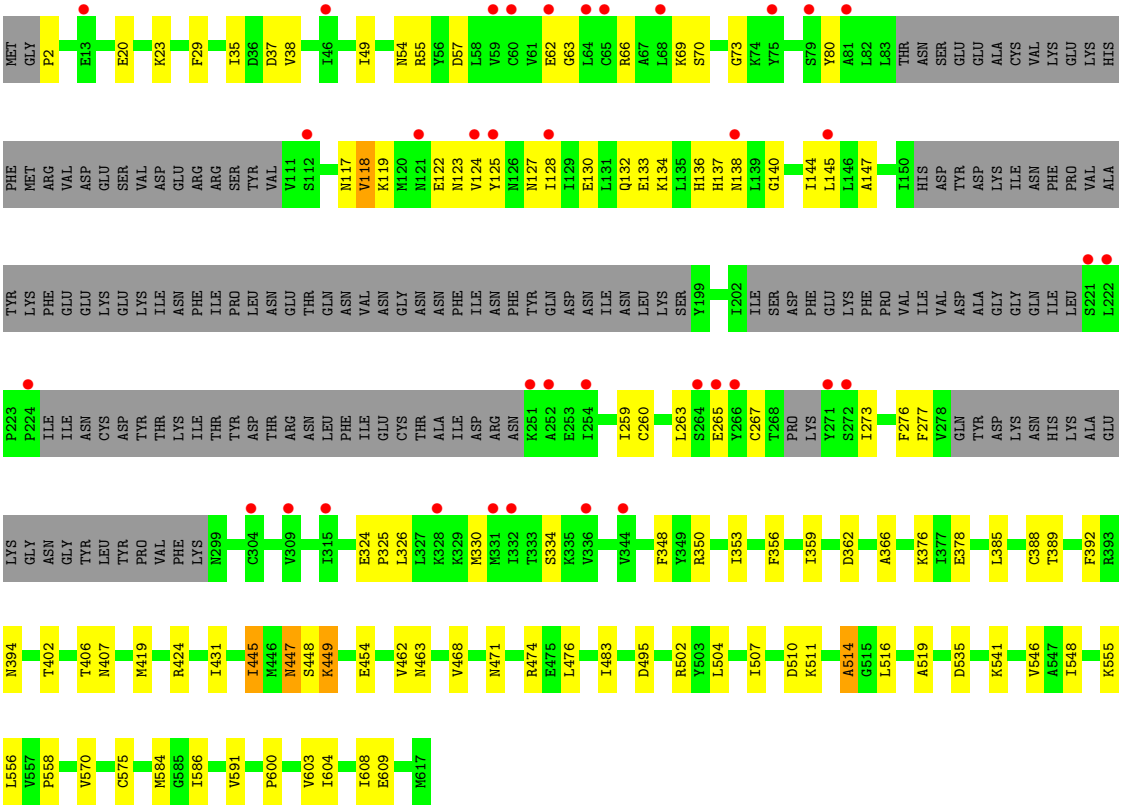
Chain B:





• Molecule 2: Phenylalanyl-tRNA synthetase beta chain, putative





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.91Å 95.21Å 181.53Å 90.00° 97.81° 90.00°	Depositor
Resolution (Å)	29.51 – 3.10 29.51 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.51-3.10) 93.3 (29.51-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.11Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.235 , 0.266 0.235 , 0.267	Depositor DCC
R_{free} test set	2018 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	12760	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: PO4, MG, W5Y

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	0.25	0/2362	0.39	0/3191
1	C	0.19	0/2351	0.35	1/3181 (0.0%)
2	B	0.36	0/4618	0.61	13/6283 (0.2%)
2	D	0.33	0/3617	0.56	6/4908 (0.1%)
All	All	0.31	0/12948	0.52	20/17563 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	80	TYR	N-CA-C	11.57	127.36	111.74
2	B	337	ILE	N-CA-C	9.51	120.70	111.67
2	B	253	GLU	N-CA-C	-8.13	102.36	111.14
2	B	159	PRO	N-CA-CB	7.34	110.96	103.25
2	B	320	VAL	N-CA-C	7.07	117.83	110.62
2	D	276	PHE	N-CA-C	7.04	119.99	108.52
2	B	514	ALA	N-CA-C	-6.98	98.66	109.76
2	D	514	ALA	N-CA-C	-6.63	98.10	108.90
2	B	157	ASN	N-CA-C	6.47	119.17	108.49
2	B	256	VAL	N-CA-C	-6.38	104.30	110.42
2	D	259	ILE	CB-CA-C	-6.30	103.91	111.97
1	C	466	ASN	N-CA-C	6.11	119.82	111.39
2	B	321	LYS	N-CA-C	5.94	117.75	111.28
2	B	217	GLY	N-CA-C	5.63	123.89	113.76
2	D	448	SER	N-CA-C	5.48	118.80	111.24
2	B	336	VAL	CB-CA-C	-5.44	103.69	111.31
2	B	448	SER	N-CA-C	5.30	117.06	111.28
2	B	213	VAL	N-CA-C	5.11	119.97	109.34
2	D	277	PHE	N-CA-C	-5.03	99.74	109.24
2	B	305	HIS	N-CA-C	5.01	117.14	110.53

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	2298	0	2205	59	0
1	C	2286	0	2175	52	0
2	B	4537	0	4043	91	0
2	D	3559	0	3275	72	0
3	A	34	0	0	2	0
3	C	34	0	0	3	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	12760	0	11698	253	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 (253) 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:482:TYR:CD2	2:B:379:ILE:HG21	2.08	0.89
2:D:476:LEU:HD13	2:D:510:ASP:OD1	1.75	0.86
2:D:263:LEU:CD2	2:D:267:CYS:SG	2.64	0.86
2:D:263:LEU:HD23	2:D:267:CYS:SG	2.24	0.77
2:B:159:PRO:CB	2:B:215:ALA:HB2	2.15	0.77
1:A:482:TYR:CE2	2:B:379:ILE:HG21	2.20	0.75
2:D:263:LEU:HD22	2:D:267:CYS:SG	2.27	0.75
2:D:122:GLU:HA	2:D:125:TYR:HB3	1.67	0.75
2:D:389:THR:HG21	2:D:502:ARG:HD2	1.71	0.73
2:B:312:LEU:O	2:B:312:LEU:HD12	1.89	0.72
2:D:118:VAL:HG12	2:D:118:VAL:O	1.89	0.71
1:A:302:ASN:HB2	2:D:402:THR:HG23	1.71	0.70
1:C:463:ILE:HG13	1:C:539:VAL:HG22	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:556:LEU:HB3	2:B:570:VAL:HG11	1.74	0.69
1:A:482:TYR:CE2	2:B:379:ILE:CG2	2.76	0.69
1:C:497:TYR:HE2	3:C:601:W5Y:CE1	2.06	0.68
2:B:584:MET:HG3	2:B:604:ILE:HG12	1.75	0.67
1:A:508:HIS:CE1	1:A:556:ILE:O	2.47	0.67
2:B:151:HIS:HE1	2:B:227:ASN:HB3	1.59	0.67
2:D:35:ILE:HA	2:D:49:ILE:HG22	1.77	0.66
2:B:402:THR:HG23	1:C:302:ASN:HB2	1.79	0.65
1:C:463:ILE:CG1	1:C:539:VAL:HG22	2.26	0.65
1:A:522:ILE:HG12	1:A:540:ILE:HG22	1.78	0.64
2:D:584:MET:HG3	2:D:604:ILE:HG12	1.80	0.64
1:A:452:LEU:O	3:A:601:W5Y:N6	2.31	0.63
2:D:514:ALA:HB2	2:D:600:PRO:HB2	1.80	0.63
2:B:468:VAL:HG21	2:B:507:ILE:HG21	1.81	0.63
1:A:327:THR:HB	1:A:406:ARG:HH12	1.65	0.62
1:C:366:GLU:OE1	1:C:401:LYS:NZ	2.32	0.62
2:B:559:LYS:HE3	2:B:561:ASP:HB2	1.82	0.62
2:B:176:ASN:OD1	2:B:232:LYS:NZ	2.33	0.62
1:A:508:HIS:HE1	1:A:556:ILE:O	1.82	0.61
1:C:344:PRO:HG3	1:C:391:TRP:CE2	2.35	0.61
1:C:504:VAL:HG23	1:C:517:VAL:HG23	1.82	0.61
1:C:327:THR:HB	1:C:406:ARG:HH12	1.66	0.61
1:A:328:HIS:NE2	2:D:609:GLU:OE2	2.26	0.59
2:D:424:ARG:HH11	2:D:431:ILE:HG22	1.68	0.59
2:D:447:ASN:OD1	2:D:447:ASN:N	2.36	0.59
1:C:314:LYS:HG2	1:C:436:PHE:HE2	1.67	0.58
2:D:136:HIS:NE2	2:D:147:ALA:HA	2.17	0.58
2:D:69:LYS:O	2:D:73:GLY:N	2.37	0.57
2:D:507:ILE:HG12	2:D:603:VAL:HG23	1.85	0.57
2:D:556:LEU:HB3	2:D:570:VAL:HG11	1.85	0.57
1:A:548:ARG:HG2	1:A:551:MET:HE2	1.85	0.57
1:C:350:ARG:NH1	1:C:353:GLN:OE1	2.37	0.57
2:B:102:SER:HB3	2:B:164:PHE:HB2	1.86	0.56
2:D:2:PRO:HG2	2:D:138:ASN:ND2	2.20	0.56
2:B:314:GLY:O	2:B:372:ILE:HD11	2.05	0.56
1:C:410:THR:O	1:C:413:SER:HB2	2.06	0.56
2:D:462:VAL:HG23	2:D:463:ASN:H	1.69	0.56
2:D:117:ASN:C	2:D:119:LYS:H	2.14	0.55
2:D:476:LEU:CD1	2:D:510:ASP:OD1	2.52	0.55
1:A:335:PHE:HA	1:A:339:ASP:HB2	1.88	0.55
2:B:309:VAL:HG13	2:B:360:VAL:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:342:PHE:CD1	2:B:342:PHE:C	2.85	0.55
2:D:130:GLU:O	2:D:134:LYS:HB2	2.06	0.55
2:D:118:VAL:O	2:D:118:VAL:CG1	2.54	0.55
2:B:308:TYR:CD1	2:B:308:TYR:C	2.85	0.54
2:B:304:CYS:CB	2:B:356:PHE:CZ	2.91	0.54
2:B:97:MET:HA	2:B:160:VAL:O	2.08	0.54
2:D:124:VAL:O	2:D:127:ASN:N	2.40	0.54
2:B:6:VAL:HG22	2:B:61:VAL:HB	1.89	0.54
2:B:514:ALA:HB2	2:B:600:PRO:HB2	1.88	0.54
2:D:330:MET:HG3	2:D:362:ASP:HB3	1.90	0.54
2:B:406:THR:HB	2:B:463:ASN:HB3	1.91	0.53
2:D:124:VAL:O	2:D:128:ILE:N	2.33	0.53
2:D:471:ASN:HB3	2:D:474:ARG:HG3	1.91	0.53
1:A:311:ARG:NH2	2:D:394:ASN:OD1	2.38	0.53
1:A:376:ASN:OD1	1:A:379:ARG:NH2	2.41	0.53
1:A:497:TYR:HD1	1:A:498:THR:HG23	1.73	0.53
1:A:306:LEU:HD21	1:A:562:LEU:HD23	1.92	0.52
2:B:254:ILE:O	2:B:258:ILE:N	2.37	0.52
2:B:324:GLU:N	2:B:325:PRO:HD2	2.25	0.52
2:B:419:MET:HE3	2:B:591:VAL:HG11	1.92	0.52
1:C:344:PRO:HB2	1:C:347:HIS:HB2	1.90	0.52
1:A:304:HIS:HB3	1:A:307:ILE:HG12	1.91	0.52
2:B:350:ARG:HH21	2:B:353:ILE:HD11	1.74	0.52
2:B:445:ILE:O	1:C:359:LYS:N	2.43	0.51
1:A:494:PHE:CZ	2:B:54:ASN:HB3	2.45	0.51
2:B:130:GLU:O	2:B:134:LYS:HB2	2.10	0.51
2:B:410:LEU:HD11	2:B:415:ASN:HB2	1.92	0.51
2:D:140:GLY:O	2:D:144:ILE:N	2.43	0.51
2:D:140:GLY:O	2:D:145:LEU:N	2.34	0.51
2:B:167:LYS:HD3	2:B:184:ASN:HA	1.92	0.51
2:B:450:THR:HG22	2:B:452:GLU:H	1.76	0.51
1:C:493:THR:HG22	1:C:494:PHE:H	1.76	0.50
2:B:449:LYS:O	2:B:449:LYS:HG2	2.10	0.50
2:B:175:LEU:HD23	2:B:176:ASN:CG	2.36	0.50
1:A:344:PRO:O	1:A:350:ARG:HD3	2.12	0.50
1:A:345:GLN:HE21	1:A:395:TRP:CD1	2.30	0.50
1:A:475:THR:HA	2:B:377:ILE:HD11	1.93	0.50
1:A:366:GLU:OE2	1:A:401:LYS:NZ	2.32	0.49
2:B:187:ILE:O	2:B:191:GLN:HG2	2.12	0.49
1:A:353:GLN:HB3	1:A:443:ARG:HH21	1.78	0.49
2:B:541:LYS:HG3	2:B:548:ILE:HD11	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:TYR:HA	2:D:128:ILE:HG12	1.93	0.49
2:B:342:PHE:HD1	2:B:342:PHE:O	1.96	0.49
2:B:67:ALA:HA	2:B:331:MET:SD	2.51	0.49
2:D:385:LEU:O	2:D:389:THR:HG23	2.12	0.49
1:A:472:LEU:HD13	1:A:540:ILE:HB	1.94	0.49
2:B:444:GLN:HE21	1:C:360:VAL:HG22	1.78	0.49
1:C:489:ARG:HB3	2:D:29:PHE:CZ	2.48	0.49
2:B:385:LEU:O	2:B:389:THR:HG23	2.12	0.49
2:B:135:LEU:HD23	2:B:255:ALA:HB1	1.94	0.49
2:D:132:GLN:C	2:D:134:LYS:H	2.21	0.49
2:B:55:ARG:HH21	2:B:350:ARG:HD3	1.78	0.49
1:A:298:MET:SD	2:B:518:GLU:HG3	2.54	0.48
2:B:342:PHE:C	2:B:342:PHE:HD1	2.21	0.48
2:B:446:MET:HB3	1:C:359:LYS:HB2	1.94	0.48
1:A:314:LYS:HG3	1:A:436:PHE:CE2	2.48	0.48
2:B:574:LEU:O	2:B:578:ASN:N	2.46	0.48
1:C:325:MET:HG3	1:C:435:PHE:HB3	1.94	0.48
1:C:337:CYS:HA	1:C:411:ALA:HB2	1.94	0.48
1:A:338:PHE:HA	1:A:343:ILE:HD12	1.95	0.48
1:A:503:GLU:OE2	1:A:505:TYR:OH	2.26	0.48
1:C:335:PHE:HA	1:C:339:ASP:HB2	1.95	0.48
1:A:346:GLN:C	1:A:348:PRO:HD3	2.39	0.48
2:B:312:LEU:HD12	2:B:312:LEU:C	2.35	0.48
2:B:557:VAL:HG23	2:B:571:ASP:HB2	1.94	0.48
1:C:303:ILE:HG13	1:C:311:ARG:HH12	1.78	0.48
2:D:468:VAL:HG21	2:D:507:ILE:HG21	1.95	0.48
2:B:350:ARG:NH1	2:B:352:ASP:OD2	2.47	0.48
2:B:415:ASN:HA	2:B:462:VAL:HG11	1.96	0.48
1:C:338:PHE:HA	1:C:343:ILE:HD12	1.95	0.48
2:B:407:ASN:O	2:B:463:ASN:ND2	2.47	0.47
1:C:345:GLN:HE21	1:C:395:TRP:NE1	2.12	0.47
1:C:497:TYR:HE2	3:C:601:W5Y:CD1	2.28	0.47
1:A:385:ASP:OD1	1:A:386:TYR:N	2.45	0.47
2:B:162:TYR:HA	2:B:212:ILE:HA	1.97	0.47
2:D:117:ASN:C	2:D:119:LYS:N	2.73	0.47
1:A:422:LYS:HD2	1:A:422:LYS:HA	1.76	0.47
2:B:160:VAL:HA	2:B:213:VAL:O	2.15	0.47
1:C:356:PHE:HB2	1:C:405:LEU:HB2	1.97	0.46
1:C:345:GLN:OE1	1:C:399:SER:OG	2.31	0.46
2:B:476:LEU:HD23	2:B:511:LYS:N	2.30	0.46
1:A:337:CYS:HA	1:A:411:ALA:HB2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:TYR:HD2	1:C:498:THR:HG23	1.80	0.46
1:A:343:ILE:HG12	1:A:496:PRO:HB2	1.97	0.46
1:C:543:GLY:N	3:C:601:W5Y:CD2	2.79	0.46
1:C:385:ASP:OD1	1:C:386:TYR:N	2.46	0.46
1:C:327:THR:OG1	1:C:439:ASP:OD2	2.30	0.46
1:C:304:HIS:HB3	1:C:307:ILE:HG12	1.99	0.45
2:D:555:LYS:HD3	2:D:575:CYS:SG	2.55	0.45
1:C:447:LEU:HD22	1:C:452:LEU:HD23	1.98	0.45
1:C:495:ASN:HB2	1:C:498:THR:OG1	2.17	0.45
2:B:243:GLU:CD	2:B:243:GLU:C	2.85	0.45
2:D:419:MET:HE3	2:D:591:VAL:HG11	1.98	0.45
1:A:479:PHE:O	1:A:483:ILE:HG12	2.17	0.45
2:D:516:LEU:HD22	2:D:586:ILE:HG13	1.99	0.45
2:B:190:TYR:CG	2:B:196:LEU:HD11	2.52	0.45
1:C:335:PHE:HE1	1:C:377:VAL:HG21	1.82	0.45
1:A:353:GLN:HB3	1:A:443:ARG:NH2	2.32	0.44
2:B:132:GLN:C	2:B:134:LYS:H	2.25	0.44
1:C:438:ILE:HG12	1:C:458:VAL:HG22	1.98	0.44
2:B:507:ILE:CD1	2:B:603:VAL:HG23	2.47	0.44
2:B:445:ILE:HG22	2:B:446:MET:O	2.17	0.44
2:B:70:SER:CB	2:B:331:MET:HG2	2.47	0.44
2:D:510:ASP:OD1	2:D:511:LYS:N	2.46	0.44
1:C:494:PHE:CE1	2:D:54:ASN:HB3	2.52	0.44
1:C:558:ASN:HB3	1:C:561:ASP:OD1	2.17	0.44
2:D:445:ILE:H	2:D:445:ILE:HG12	1.57	0.44
1:A:424:TYR:CZ	1:A:534:PRO:HG3	2.53	0.44
1:A:528:LEU:HA	1:A:531:MET:HE3	1.99	0.44
1:C:419:GLN:O	1:C:422:LYS:HB2	2.18	0.44
1:A:482:TYR:CE2	2:B:379:ILE:HG22	2.53	0.44
2:B:133:GLU:HA	2:B:136:HIS:HB2	1.99	0.44
2:D:20:GLU:HB2	2:D:23:LYS:HB2	1.99	0.44
2:B:302:LEU:HG	2:B:356:PHE:CZ	2.53	0.44
1:C:322:PHE:HB3	1:C:436:PHE:HD1	1.83	0.44
1:A:533:PHE:HB3	1:A:537:VAL:HG21	2.00	0.43
1:A:348:PRO:O	2:B:53:ALA:HB1	2.18	0.43
2:B:612:MET:HE3	2:B:612:MET:HB2	1.85	0.43
1:A:345:GLN:NE2	1:A:396:GLU:H	2.16	0.43
2:B:581:PHE:HB3	2:B:610:THR:HG21	2.01	0.43
2:D:133:GLU:O	2:D:137:HIS:ND1	2.51	0.43
1:A:325:MET:HE2	1:A:435:PHE:HB3	1.99	0.43
2:B:228:CYS:SG	2:B:231:THR:OG1	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:LEU:O	2:B:395:VAL:HG23	2.18	0.43
2:B:445:ILE:HD12	2:B:453:TYR:O	2.18	0.43
2:B:350:ARG:NH2	2:B:362:ASP:OD1	2.47	0.43
2:D:356:PHE:O	2:D:359:ILE:HG12	2.18	0.43
2:B:35:ILE:HA	2:B:49:ILE:HG22	2.00	0.43
2:B:331:MET:HE2	2:B:331:MET:HB2	1.78	0.43
2:B:395:VAL:HG21	2:B:529:GLU:HG2	2.00	0.43
2:D:350:ARG:HB3	2:D:353:ILE:HG22	2.00	0.43
1:A:438:ILE:HA	1:A:457:GLN:O	2.18	0.43
1:A:482:TYR:HE2	2:B:379:ILE:HG22	1.84	0.43
1:C:463:ILE:CD1	1:C:539:VAL:HG22	2.49	0.43
1:A:525:PRO:HG2	2:B:355:HIS:CE1	2.54	0.43
2:B:507:ILE:HD13	2:B:603:VAL:HG23	2.00	0.42
2:D:388:CYS:HG	2:D:392:PHE:HE2	1.66	0.42
1:A:467:LEU:HD12	1:A:538:SER:O	2.18	0.42
2:B:462:VAL:HG23	2:B:463:ASN:H	1.84	0.42
1:A:353:GLN:CG	1:A:443:ARG:HH21	2.32	0.42
2:D:326:LEU:HD12	2:D:366:ALA:HB1	2.01	0.42
2:D:483:ILE:HB	2:D:504:LEU:HD13	2.01	0.42
2:D:263:LEU:HD23	2:D:263:LEU:HA	1.72	0.42
2:B:302:LEU:HG	2:B:356:PHE:CE2	2.55	0.42
1:C:479:PHE:O	1:C:483:ILE:HG12	2.20	0.42
2:D:62:GLU:CB	2:D:265:GLU:CB	2.98	0.42
2:D:406:THR:HB	2:D:463:ASN:HB3	2.01	0.42
1:A:314:LYS:HE3	1:A:314:LYS:HB2	1.83	0.42
1:C:489:ARG:HB3	2:D:29:PHE:HZ	1.85	0.42
2:D:63:GLY:HA2	2:D:66:ARG:NE	2.35	0.42
2:D:558:PRO:HA	2:D:570:VAL:HG22	2.02	0.42
1:A:314:LYS:HG3	1:A:436:PHE:CZ	2.55	0.42
1:C:508:HIS:ND1	1:C:511:ASN:HB2	2.35	0.42
2:B:181:VAL:HG11	2:B:186:PHE:HD2	1.84	0.41
2:D:392:PHE:CE2	2:D:608:ILE:HD12	2.56	0.41
2:D:541:LYS:HG3	2:D:548:ILE:HD11	2.02	0.41
2:B:389:THR:HG21	2:B:502:ARG:HD2	2.02	0.41
2:D:324:GLU:OE2	2:D:334:SER:HB3	2.20	0.41
2:B:31:PHE:HD2	2:B:33:ILE:HG12	1.85	0.41
2:B:403:GLU:HB2	2:B:481:PHE:CZ	2.56	0.41
1:A:438:ILE:HG12	1:A:458:VAL:HG22	2.03	0.41
2:B:535:ASP:OD1	2:B:535:ASP:N	2.54	0.41
1:C:350:ARG:O	1:C:354:ASP:HB2	2.20	0.41
1:C:498:THR:O	1:C:501:SER:OG	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:66:ARG:O	2:D:70:SER:OG	2.31	0.41
1:A:343:ILE:HG22	1:A:350:ARG:HD2	2.02	0.41
1:A:551:MET:HB2	1:A:556:ILE:HB	2.02	0.41
2:D:37:ASP:OD2	2:D:38:VAL:N	2.54	0.41
2:D:445:ILE:HG12	2:D:454:GLU:O	2.20	0.41
1:A:464:ASP:O	1:A:538:SER:O	2.38	0.41
2:B:356:PHE:O	2:B:360:VAL:HG23	2.21	0.41
2:B:611:ILE:O	2:B:615:LEU:HG	2.19	0.41
1:C:349:SER:OG	1:C:351:ASP:OD2	2.32	0.41
1:A:364:CYS:HB2	2:D:495:ASP:O	2.21	0.41
1:A:476:LEU:HD13	1:A:476:LEU:HA	1.95	0.41
2:B:386:SER:O	2:B:390:GLU:HG2	2.20	0.41
2:D:55:ARG:HB2	2:D:57:ASP:OD1	2.20	0.41
1:C:377:VAL:HA	1:C:380:VAL:HG22	2.03	0.40
1:C:508:HIS:CG	1:C:511:ASN:HB2	2.56	0.40
2:D:541:LYS:HB3	2:D:546:VAL:HB	2.02	0.40
1:A:353:GLN:CB	1:A:443:ARG:HH21	2.34	0.40
2:B:421:ARG:HG3	2:B:439:LEU:HD21	2.03	0.40
1:C:344:PRO:HB2	1:C:347:HIS:CB	2.51	0.40
2:D:407:ASN:O	2:D:463:ASN:ND2	2.52	0.40
2:D:535:ASP:N	2:D:535:ASP:OD1	2.54	0.40
1:A:354:ASP:HB3	1:A:444:ASN:HB3	2.03	0.40
1:A:397:LEU:O	1:A:400:THR:HG22	2.22	0.40
1:A:445:GLU:OE2	3:A:601:W5Y:N6	2.54	0.40
1:C:341:LEU:O	1:C:497:TYR:HB3	2.21	0.40
1:C:463:ILE:HD12	1:C:539:VAL:CG2	2.51	0.40
2:D:260:CYS:HB3	2:D:348:PHE:HE1	1.86	0.40
2:D:324:GLU:N	2:D:325:PRO:HD2	2.36	0.40
2:D:376:LYS:NZ	2:D:378:GLU:HG2	2.36	0.40
2:B:100:ASP:OD1	2:B:101:GLU:N	2.54	0.40
1:C:402:LYS:HE2	1:C:402:LYS:HB3	1.92	0.40
2:B:103:VAL:HA	2:B:164:PHE:CE2	2.56	0.40
2:B:539:GLU:OE1	2:B:543:LYS:HE2	2.21	0.40
2:D:449:LYS:HE3	2:D:449:LYS:HB2	1.80	0.40
2:D:519:ALA:O	2:D:604:ILE:HD11	2.22	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	279/299 (93%)	270 (97%)	9 (3%)	0	100	100
1	C	280/299 (94%)	272 (97%)	8 (3%)	0	100	100
2	B	606/618 (98%)	567 (94%)	36 (6%)	3 (0%)	24	57
2	D	461/618 (75%)	435 (94%)	23 (5%)	3 (1%)	18	49
All	All	1626/1834 (89%)	1544 (95%)	76 (5%)	6 (0%)	30	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	159	PRO
2	D	273	ILE
2	D	118	VAL
2	D	449	LYS
2	B	219	ILE
2	B	226	ILE

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	246/274 (90%)	245 (100%)	1 (0%)	84	86
1	C	244/274 (89%)	243 (100%)	1 (0%)	84	86
2	B	432/572 (76%)	425 (98%)	7 (2%)	55	75
2	D	353/572 (62%)	350 (99%)	3 (1%)	73	81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1275/1692 (75%)	1263 (99%)	12 (1%)	70 80

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	556	ILE
2	B	243	GLU
2	B	331	MET
2	B	337	ILE
2	B	342	PHE
2	B	379	ILE
2	B	447	ASN
2	B	513	THR
1	C	466	ASN
2	D	123	ASN
2	D	445	ILE
2	D	447	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	ASN
1	A	299	ASN
1	A	309	GLN
1	A	392	ASN
1	A	508	HIS
2	B	126	ASN
2	B	151	HIS
2	B	184	ASN
2	B	437	ASN
2	B	473	HIS
2	B	531	GLN
1	C	290	ASN
1	C	365	GLN
2	D	437	ASN
2	D	473	HIS
2	D	520	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
4	PO4	A	602	-	4,4,4	1.39	1 (25%)	6,6,6	1.09	0
3	W5Y	A	601	-	37,37,37	0.60	0	51,54,54	0.66	1 (1%)
3	W5Y	C	601	-	37,37,37	0.59	0	51,54,54	0.92	2 (3%)
4	PO4	C	602	-	4,4,4	1.36	1 (25%)	6,6,6	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	W5Y	A	601	-	-	3/22/39/39	0/4/4/4
3	W5Y	C	601	-	-	4/22/39/39	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	602	PO4	P-O1	2.39	1.56	1.50
4	A	602	PO4	P-O1	2.33	1.56	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	601	W5Y	C-NAT-SBI	-5.68	115.41	124.61
3	A	601	W5Y	C-NAT-SBI	-2.84	120.02	124.61
3	C	601	W5Y	O-C-NAT	-2.05	119.05	123.00

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	W5Y	O-C-CA-CB
3	A	601	W5Y	NAT-C-CA-CB
3	A	601	W5Y	C-NAT-SBI-OAE
3	C	601	W5Y	O-C-CA-CB
3	C	601	W5Y	NAT-C-CA-CB
3	C	601	W5Y	C5'-O5'-SBI-NAT
3	C	601	W5Y	N-CA-CB-CG

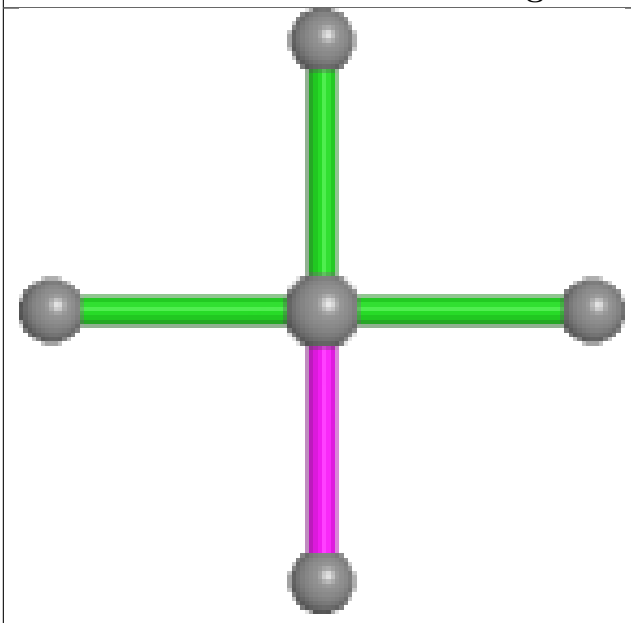
There are no ring outliers.

2 monomers are involved in 5 short contacts:

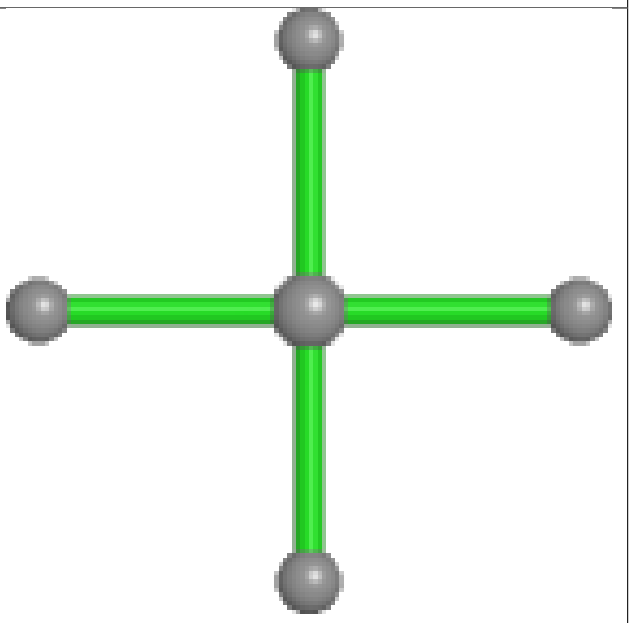
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	W5Y	2	0
3	C	601	W5Y	3	0

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

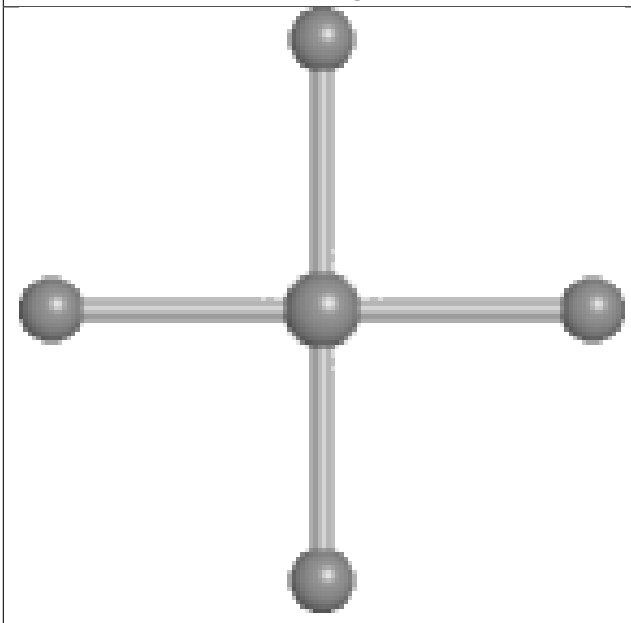
Ligand PO4 A 602



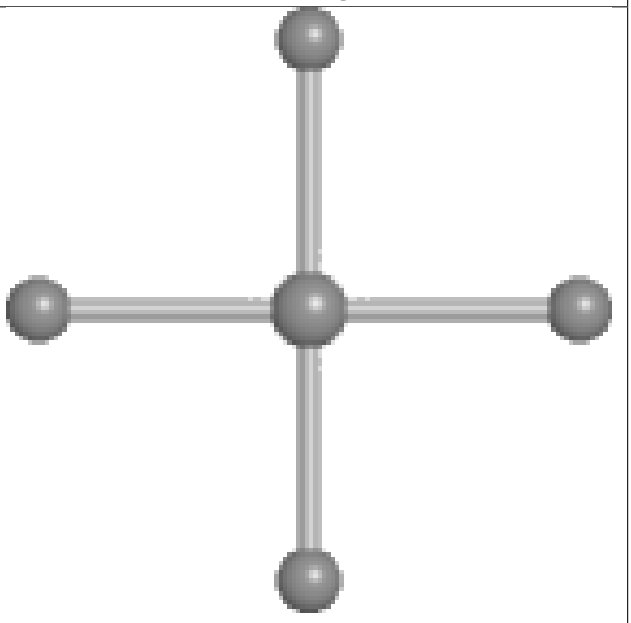
Bond lengths



Bond angles

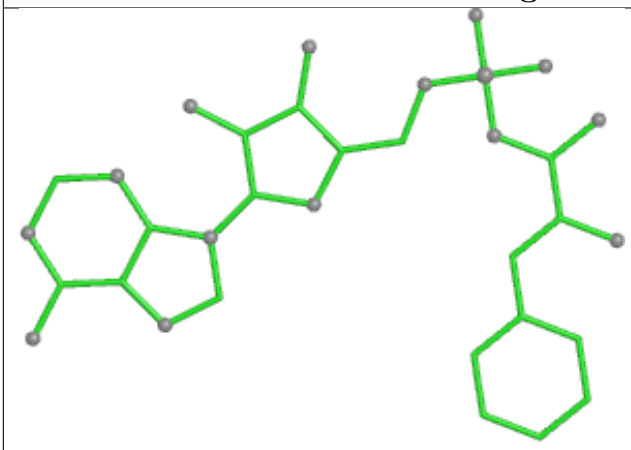


Torsions

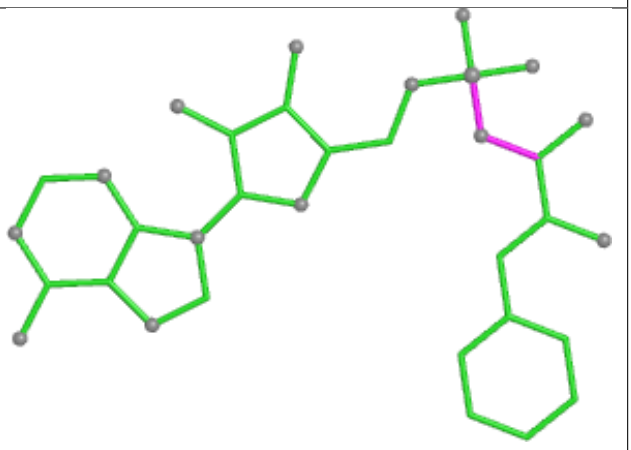


Rings

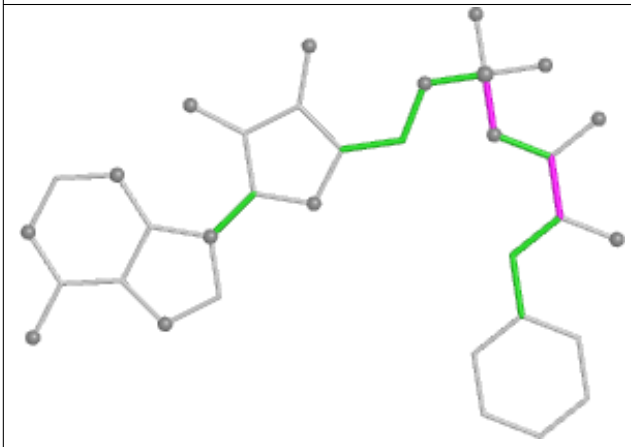
Ligand W5Y A 601



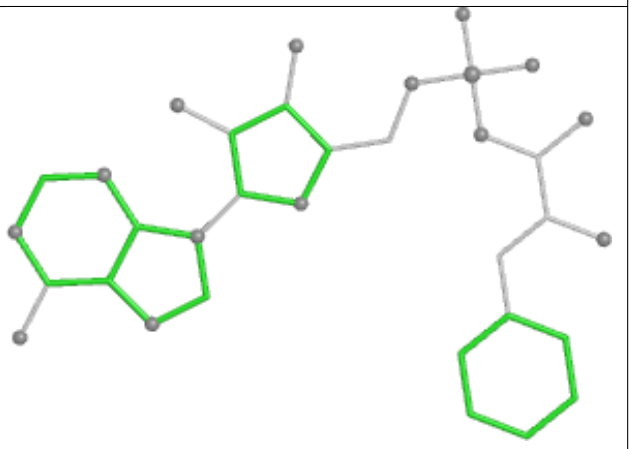
Bond lengths



Bond angles

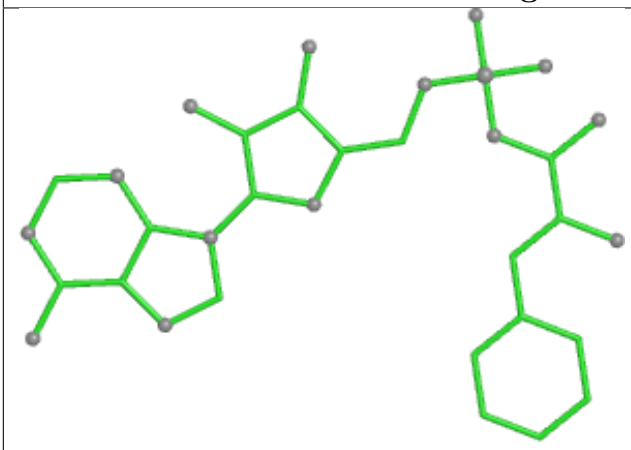


Torsions

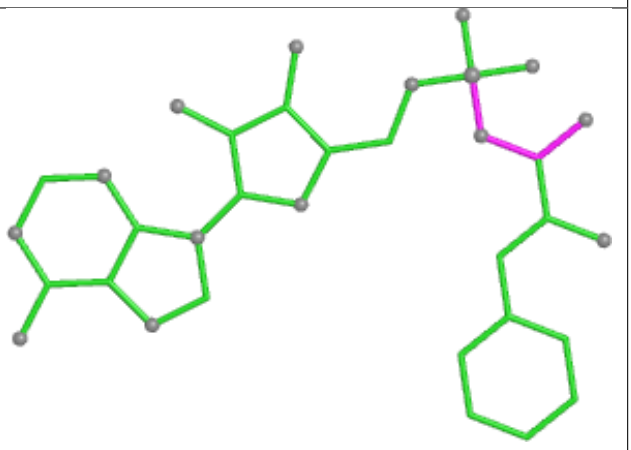


Rings

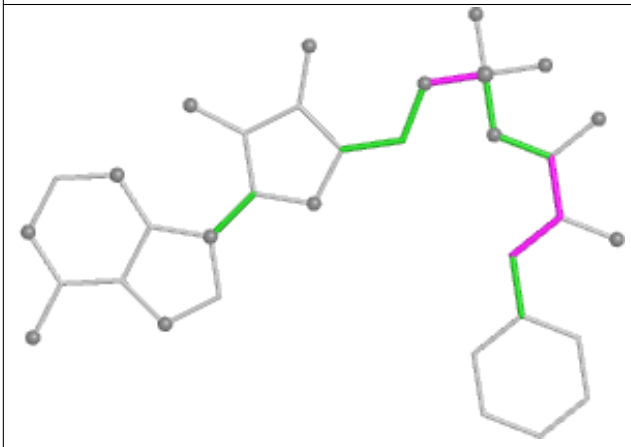
Ligand W5Y C 601



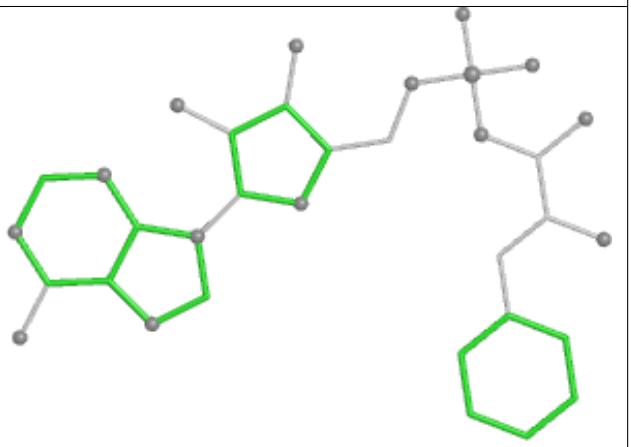
Bond lengths



Bond angles

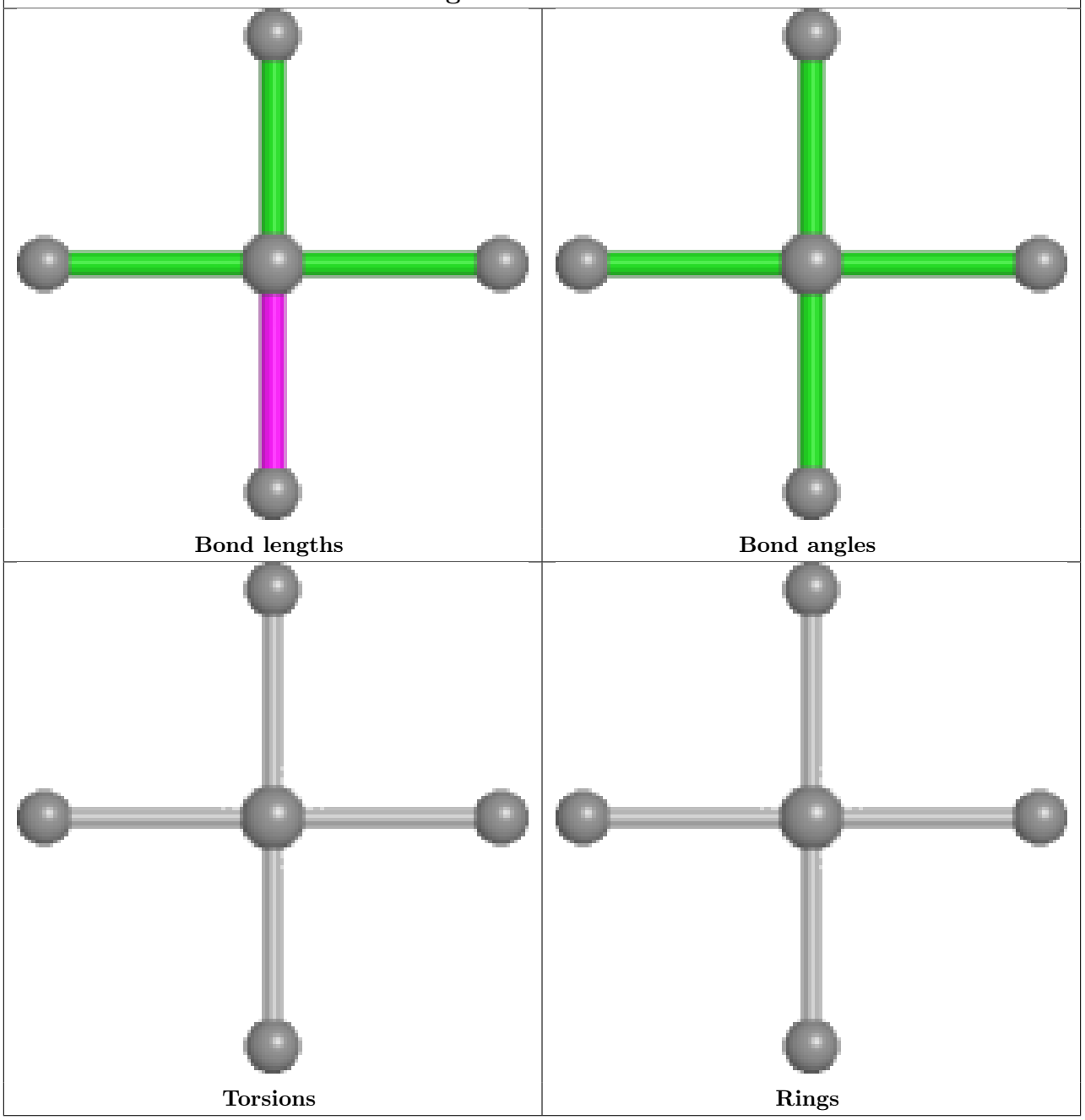


Torsions



Rings

Ligand PO4 C 602



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	281/299 (93%)	0.16	3 (1%)	78	59	46, 87, 133, 159	0
1	C	282/299 (94%)	0.08	7 (2%)	58	37	45, 80, 129, 159	0
2	B	612/618 (99%)	0.34	26 (4%)	40	22	43, 115, 170, 212	0
2	D	475/618 (76%)	0.41	37 (7%)	19	10	43, 97, 166, 224	0
All	All	1650/1834 (89%)	0.28	73 (4%)	39	21	43, 95, 160, 224	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	319	SER	5.3
2	D	221	SER	4.2
2	D	60	CYS	4.0
2	B	211	VAL	3.9
2	B	157	ASN	3.6
1	C	430	ILE	3.6
2	B	272	SER	3.6
2	D	266	TYR	3.4
2	D	309	VAL	3.3
2	B	294	TYR	3.3
2	B	103	VAL	3.3
2	D	251	LYS	3.2
2	D	315	ILE	3.1
2	D	79	SER	3.1
2	D	264	SER	3.1
2	B	268	THR	3.0
1	C	352	LEU	3.0
2	D	336	VAL	3.0
2	B	252	ALA	3.0
2	B	88	GLU	2.9
1	C	567	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	214	ASP	2.9
2	D	121	ASN	2.9
2	D	112	SER	2.8
2	D	68	LEU	2.8
2	D	75	TYR	2.7
2	D	125	TYR	2.7
1	A	347	HIS	2.7
2	D	272	SER	2.7
2	B	182	ASN	2.7
2	D	304	CYS	2.7
2	B	178	THR	2.6
2	D	254	ILE	2.6
2	D	328	LYS	2.6
2	B	369	TYR	2.6
2	B	71	PHE	2.6
2	D	128	ILE	2.5
2	D	65	CYS	2.5
1	C	354	ASP	2.5
2	D	252	ALA	2.5
2	B	295	PRO	2.4
2	D	138	ASN	2.4
2	D	59	VAL	2.4
2	B	84	THR	2.4
2	D	64	LEU	2.4
2	D	62	GLU	2.3
2	B	108	SER	2.3
2	D	332	ILE	2.3
1	C	348	PRO	2.3
2	B	161	ALA	2.3
2	D	13	GLU	2.3
2	B	156	ILE	2.3
1	C	393	TYR	2.3
2	D	265	GLU	2.2
2	B	210	PRO	2.2
2	B	266	TYR	2.2
2	B	181	VAL	2.2
2	D	124	VAL	2.2
2	B	62	GLU	2.2
2	B	207	GLU	2.2
2	B	224	PRO	2.2
1	A	427	THR	2.2
2	D	271	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	344	VAL	2.2
2	D	81	ALA	2.2
2	D	222	LEU	2.1
2	D	224	PRO	2.1
1	C	349	SER	2.1
2	D	46	ILE	2.0
2	D	331	MET	2.0
2	D	145	LEU	2.0
1	A	360	VAL	2.0
2	B	187	ILE	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 oligosaccharides in this entry.

6.4 Ligands (i)

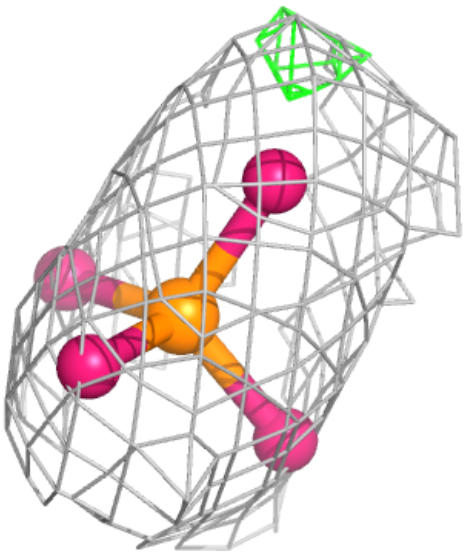
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

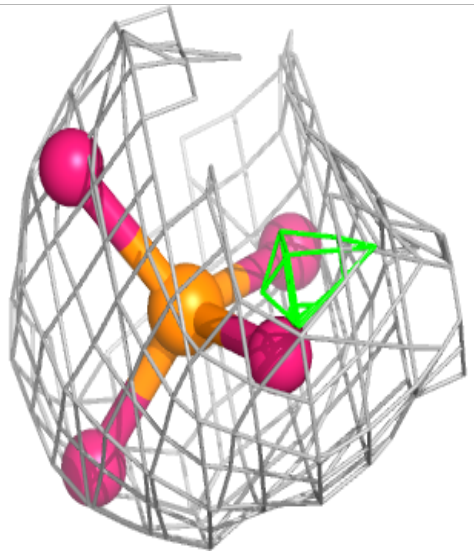
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	A	602	5/5	0.77	0.16	89,106,112,122	5
5	MG	B	701	1/1	0.82	0.28	100,100,100,100	0
5	MG	C	603	1/1	0.87	0.27	78,78,78,78	0
4	PO4	C	602	5/5	0.88	0.18	93,94,95,113	5
3	W5Y	A	601	34/34	0.94	0.10	53,70,87,89	0
3	W5Y	C	601	34/34	0.94	0.10	38,57,74,87	0

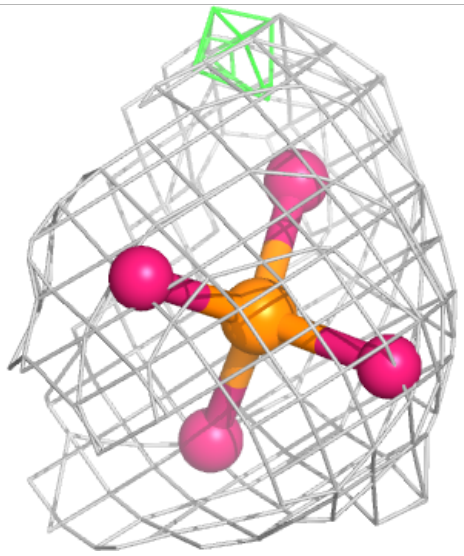
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PO4 A 602:

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

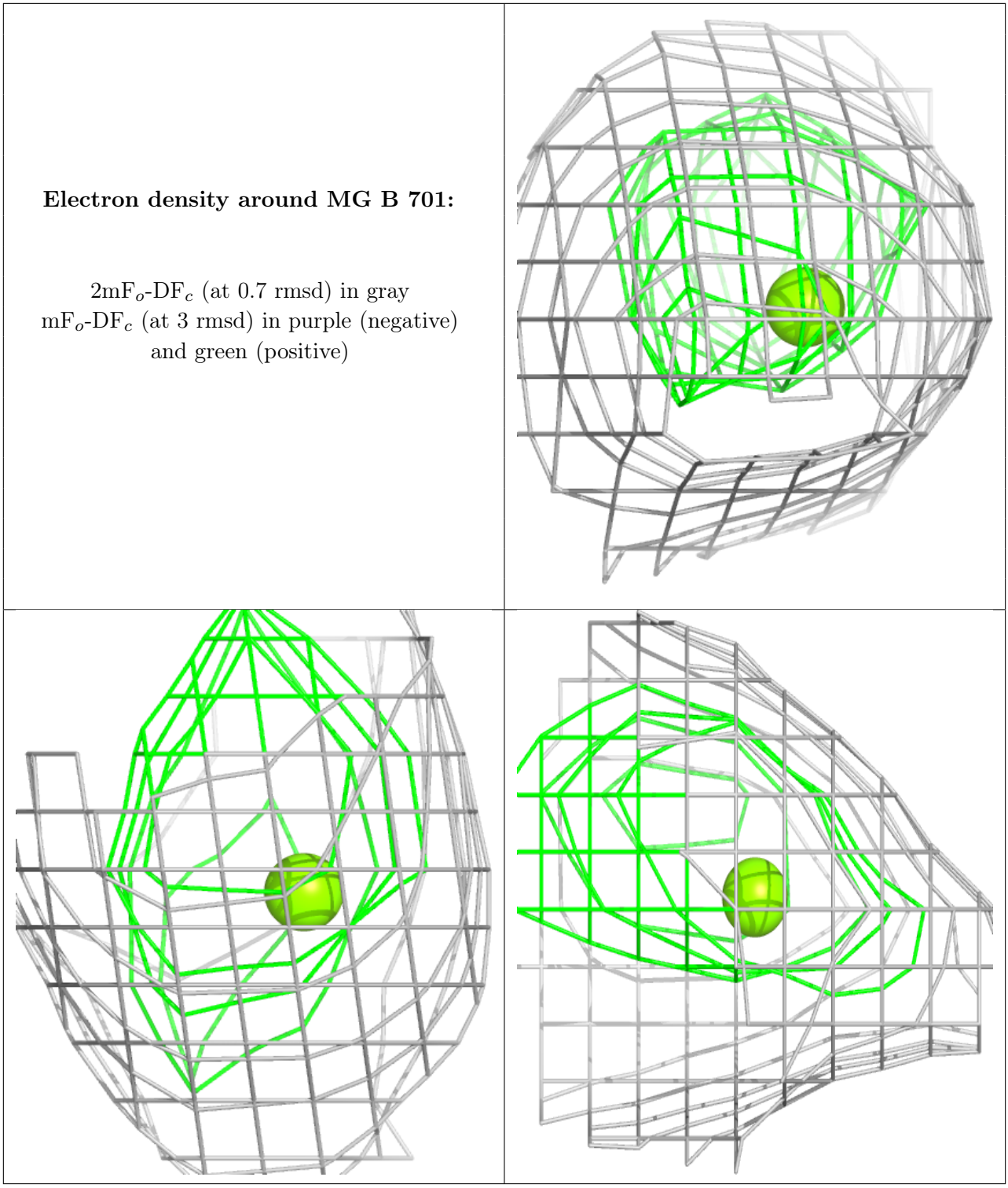






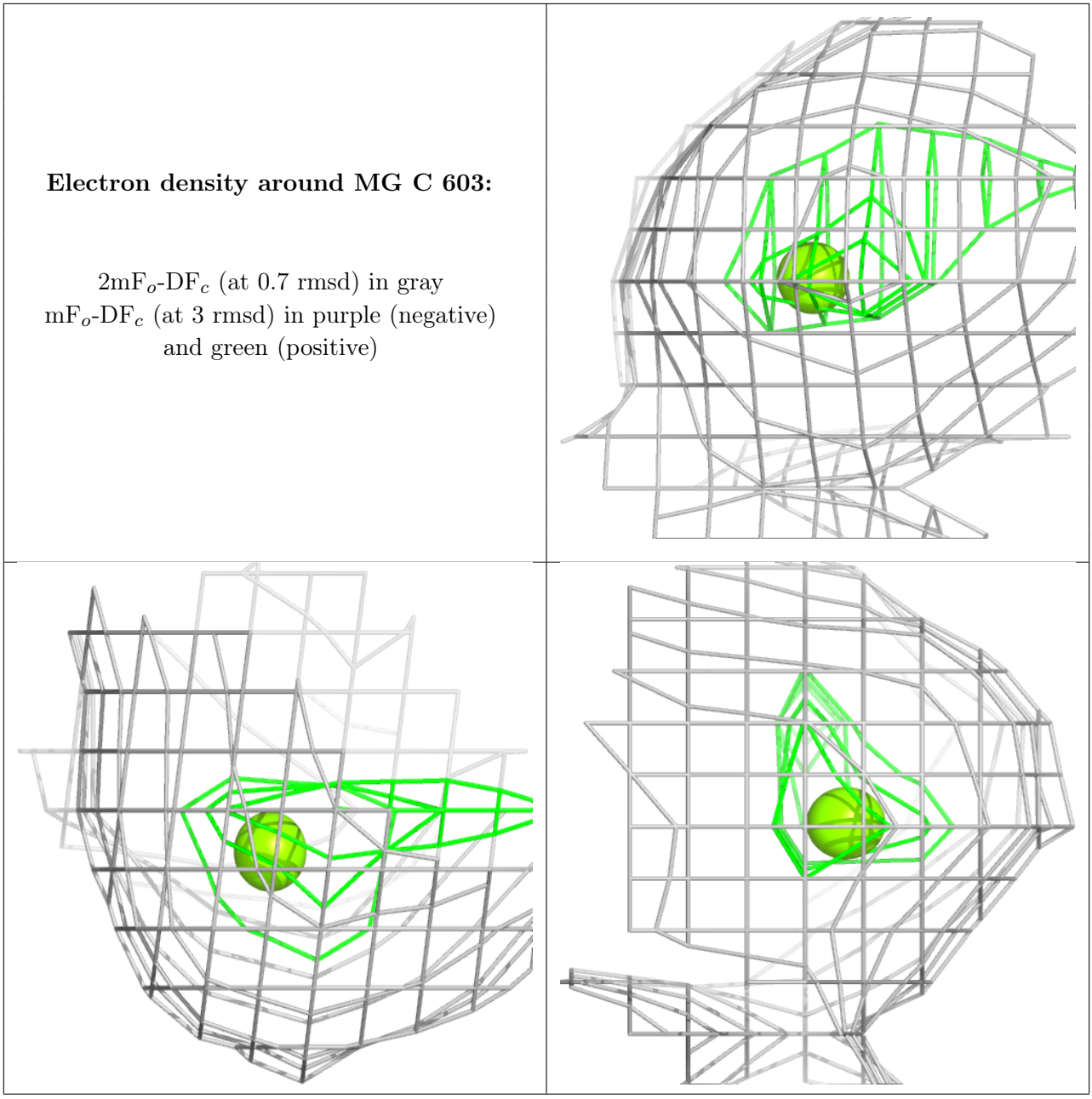
Electron density around MG B 701:

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



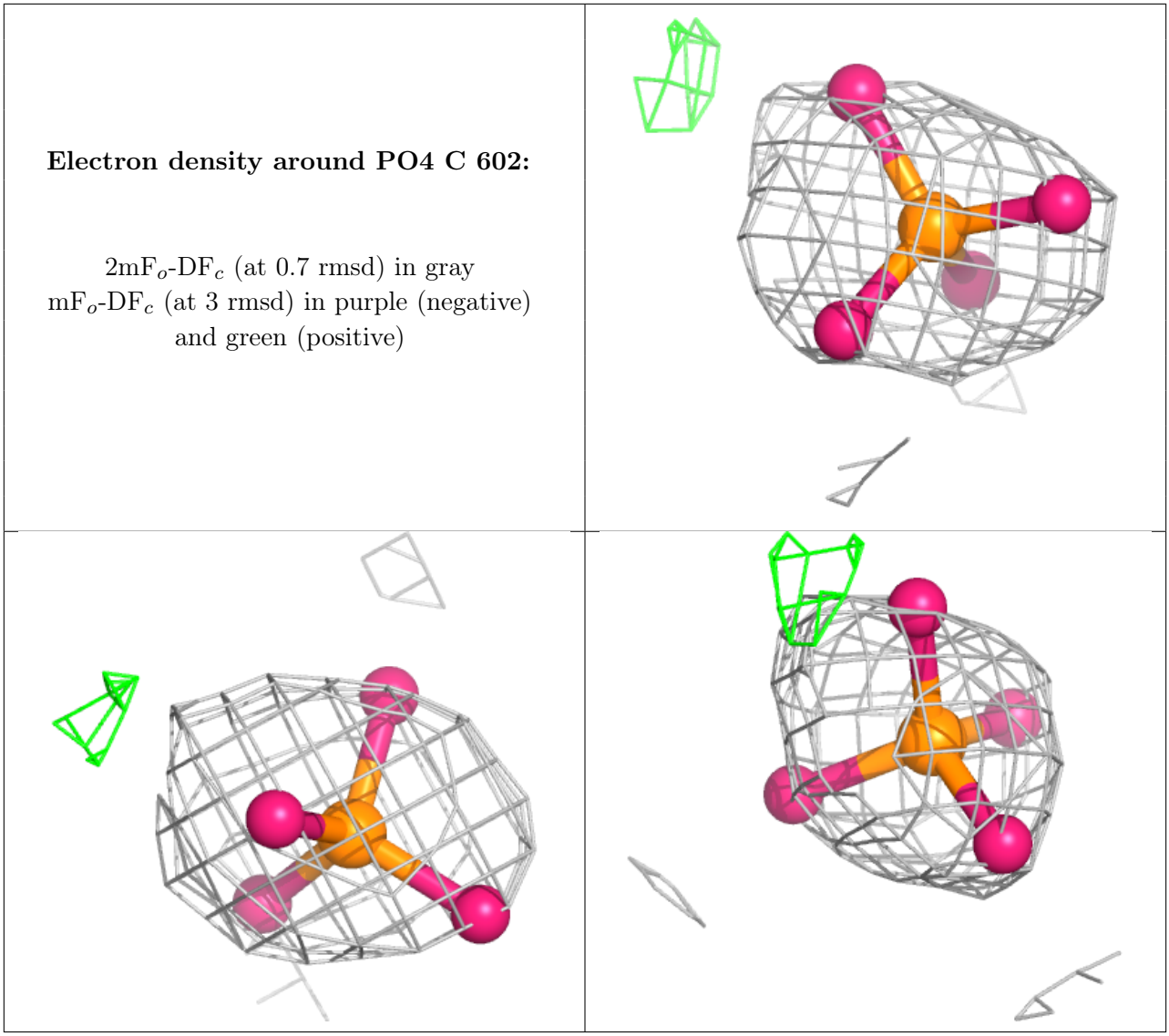
Electron density around MG C 603:

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



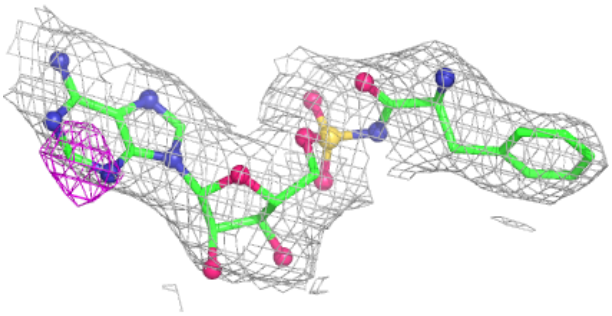
Electron density around PO4 C 602:

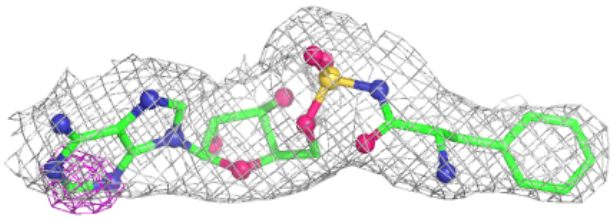
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

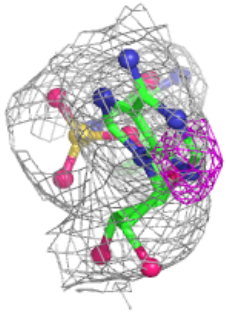


Electron density around W5Y A 601:

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

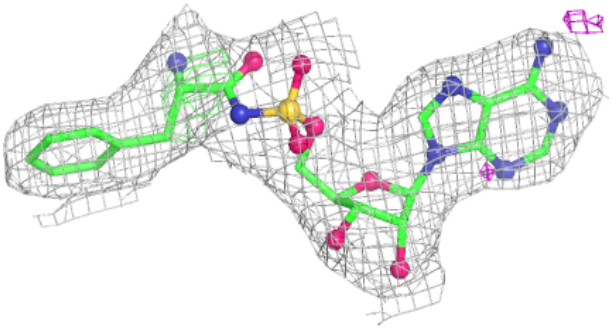


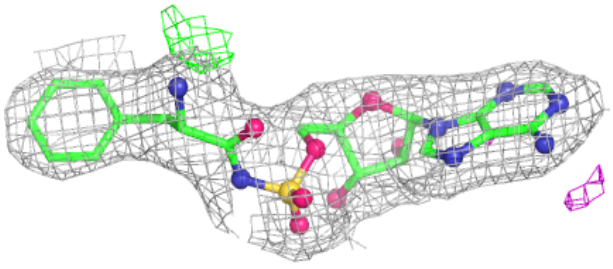


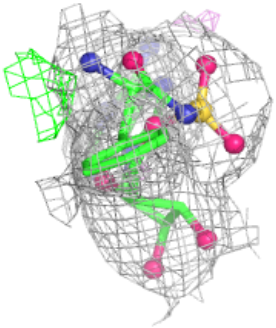


Electron density around W5Y C 601:

$2mF_o$-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.