Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2026 – 10:14 am BST

PDB ID	:	4AAY / pdb_00004aay
Title	:	Crystal Structure of the arsenite oxidase protein complex from Rhizobium species strain NT-26
Authors	:	Oke, M.; Santini, J.M.; Naismith, J.H.
Deposited on	:	2011-12-05
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

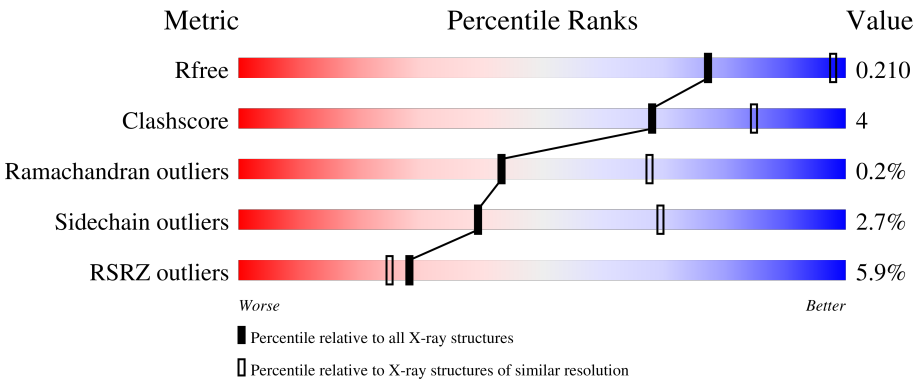
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	845	3% 92% 7%
1	C	845	4% 90% 9% •
1	E	845	4% 91% 8%
1	G	845	4% 92% 7%
2	B	175	9% 70% 5% • 25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	175	19% 67% 6% 25%
2	F	175	8% 70% 5% 25%
2	H	175	20% 68% 5% 25%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 30609 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.

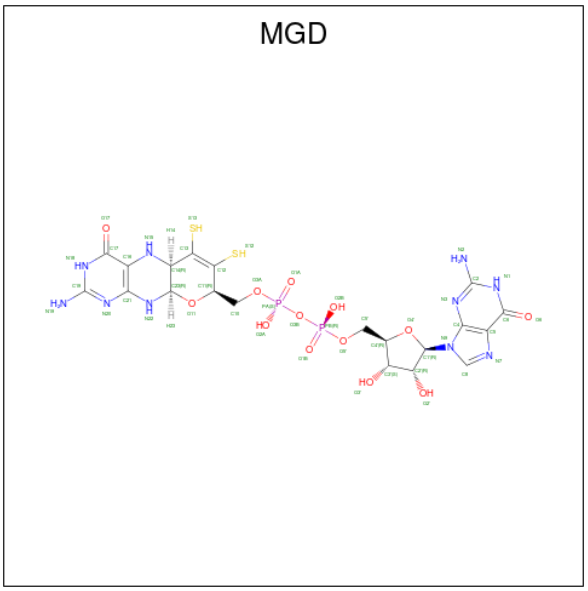
- Molecule 1 is a protein called AROA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	843	6545	4088	1167	1253	37	0	0	0
1	C	843	6551	4092	1168	1254	37	0	1	0
1	E	843	6545	4088	1167	1253	37	0	0	0
1	G	843	6545	4088	1167	1253	37	0	0	0

- Molecule 2 is a protein called AROB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	132	995	629	166	198	2	0	0	0
2	D	132	995	629	166	198	2	0	0	0
2	F	132	995	629	166	198	2	0	0	0
2	H	132	995	629	166	198	2	0	0	0

- Molecule 3 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	47	20	10	13	2	2	0	0
3	A	1	47	20	10	13	2	2	0	0
3	C	1	47	20	10	13	2	2	0	0
3	C	1	47	20	10	13	2	2	0	0
3	E	1	47	20	10	13	2	2	0	0
3	E	1	47	20	10	13	2	2	0	0
3	G	1	47	20	10	13	2	2	0	0
3	G	1	47	20	10	13	2	2	0	0

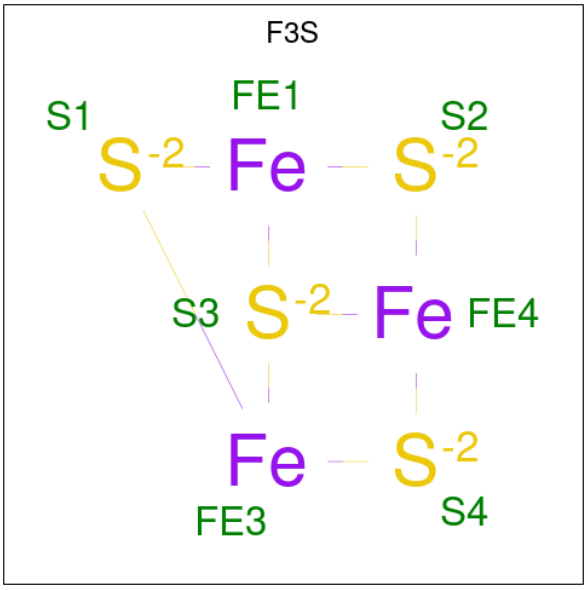
- Molecule 4 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	1	1	0	0
4	C	1	1	1	0	0
4	E	1	1	1	0	0
4	G	1	1	1	0	0

- Molecule 5 is MOLYBDENUM(IV) ION (CCD ID: 4MO) (formula: Mo).

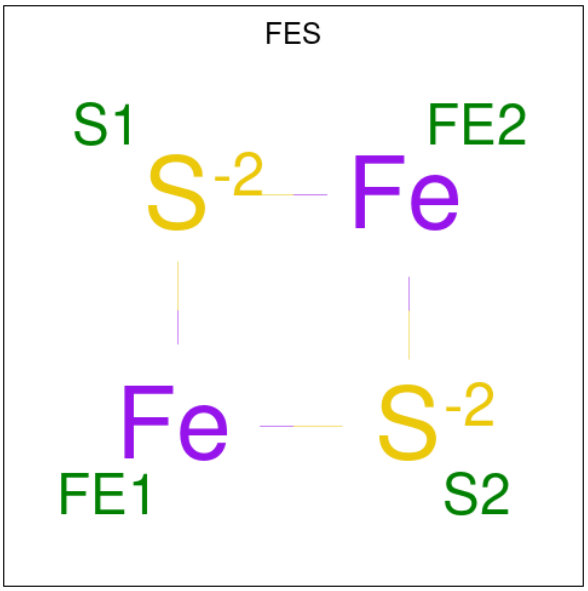
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
5	A	1	1	1	0	0
5	C	1	1	1	0	0
5	E	1	1	1	0	0
5	G	1	1	1	0	0

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
6	A	1	7	3	4	0	0
6	C	1	7	3	4	0	0
6	E	1	7	3	4	0	0
6	G	1	7	3	4	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0
7	D	1	4	2	2	0	0
7	F	1	4	2	2	0	0
7	H	1	4	2	2	0	0

- Molecule 8 is water.

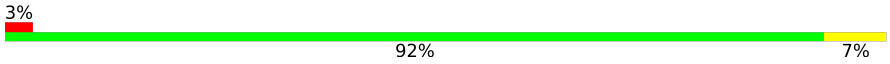
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	6	6	6	0	0
8	C	2	2	2	0	0
8	E	5	5	5	0	0
8	G	2	2	2	0	0

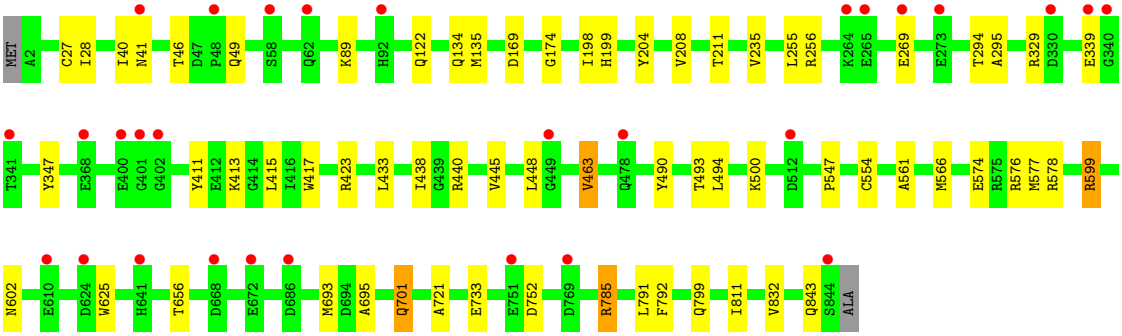
3 Residue-property plots (i)

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: AROA

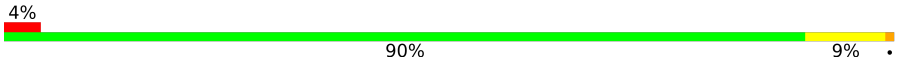
Chain A:

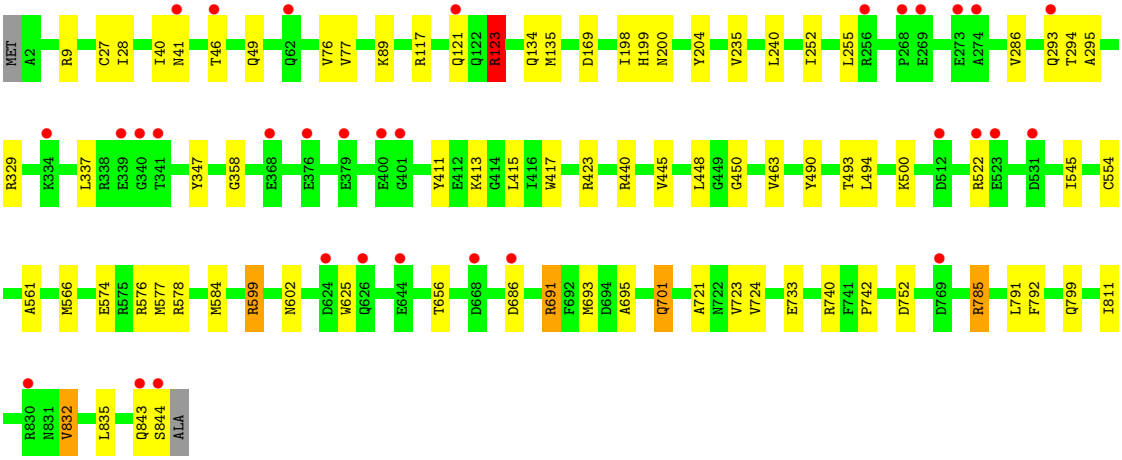




- Molecule 1: AROA

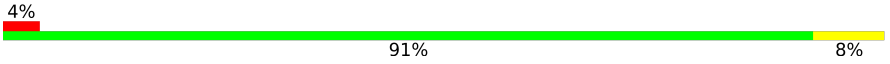
Chain C:

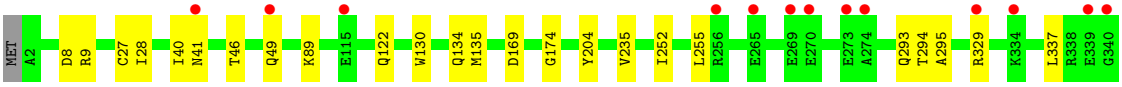


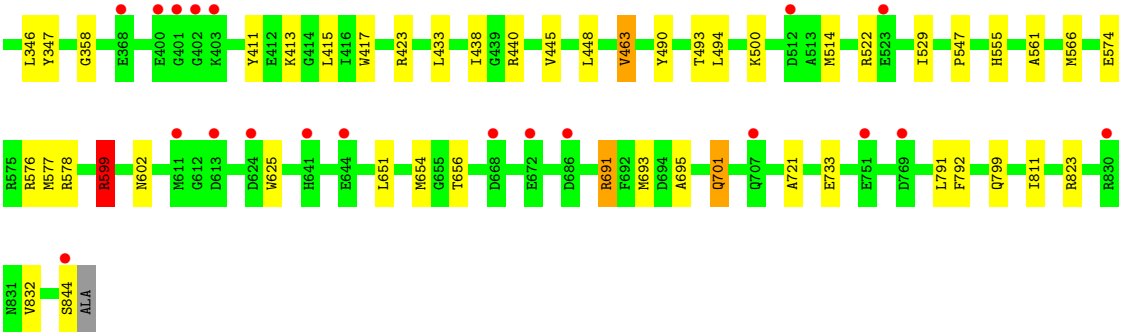


- Molecule 1: AROA

Chain E:

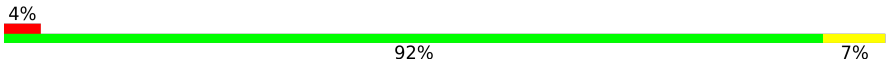


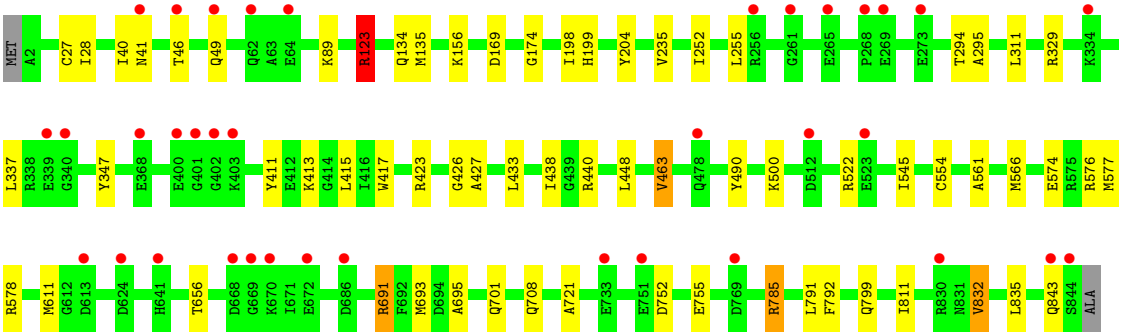




• Molecule 1: AROA

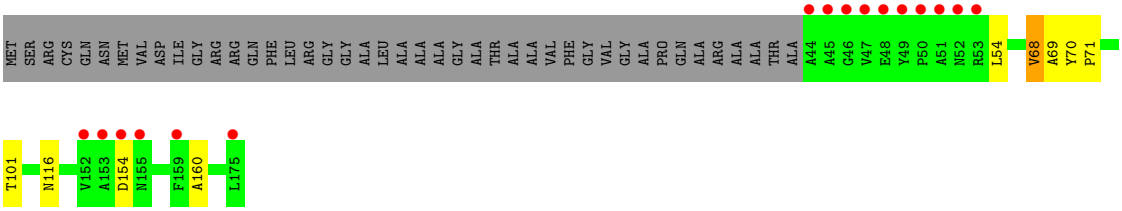
Chain G:





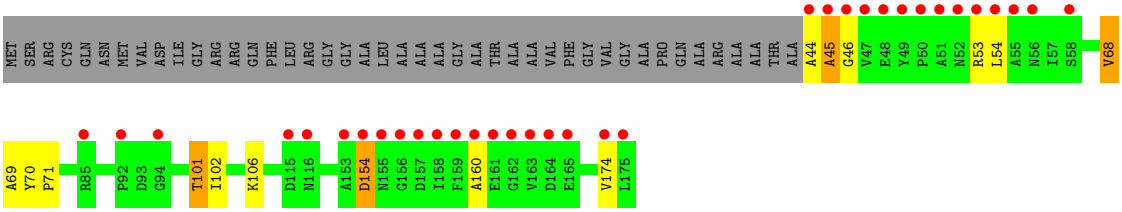
• Molecule 2: AROB

Chain B:



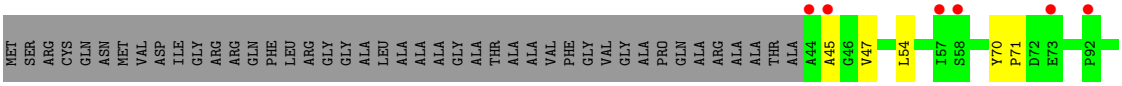
• Molecule 2: AROB

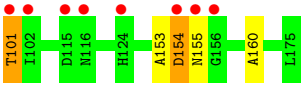
Chain D:



• Molecule 2: AROB

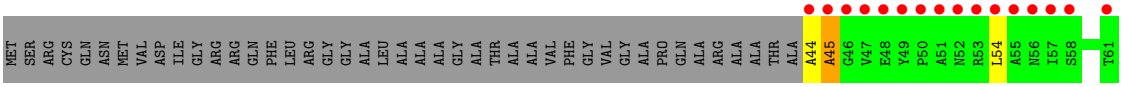
Chain F:

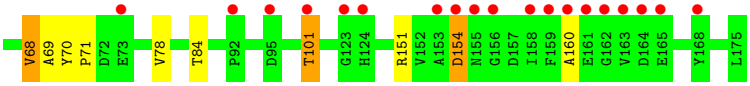




- Molecule 2: AROB

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	149.13Å 232.96Å 141.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.87 – 2.70 141.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (141.87-2.70) 99.9 (141.87-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0119	Depositor
R, R_{free}	0.193 , 0.211 0.193 , 0.210	Depositor DCC
R_{free} test set	6818 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 32.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	30609	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: O, F3S, 4MO, MGD, FES

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	0.81	0/6693	0.82	0/9068
1	C	0.79	0/6702	0.82	2/9080 (0.0%)
1	E	0.79	1/6693 (0.0%)	0.82	1/9068 (0.0%)
1	G	0.79	0/6693	0.82	1/9068 (0.0%)
2	B	0.64	0/1018	0.74	0/1387
2	D	0.66	0/1018	0.80	2/1387 (0.1%)
2	F	0.69	0/1018	0.75	0/1387
2	H	0.70	1/1018 (0.1%)	0.77	1/1387 (0.1%)
All	All	0.78	2/30853 (0.0%)	0.81	7/41832 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	2
2	F	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	151	ARG	C-N	-7.28	1.24	1.33
1	E	555	HIS	CG-CD2	5.01	1.41	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	151	ARG	O-C-N	-6.81	115.09	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	46	GLY	N-CA-C	-6.22	98.45	113.18
1	C	123	ARG	CB-CG-CD	5.99	125.06	111.30
1	G	123	ARG	CB-CG-CD	5.84	124.73	111.30
1	E	599	ARG	CD-NE-CZ	5.51	132.11	124.40
1	C	134	GLN	CB-CA-C	-5.24	99.49	111.95
2	D	53	ARG	CB-CA-C	-5.16	101.63	109.89

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	44	ALA	Peptide
2	D	45	ALA	Peptide
2	F	153	ALA	Peptide

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	6545	0	6296	45	0
1	C	6551	0	6304	49	1
1	E	6545	0	6296	57	0
1	G	6545	0	6296	43	0
2	B	995	0	947	5	0
2	D	995	0	947	15	0
2	F	995	0	947	5	0
2	H	995	0	947	8	0
3	A	94	0	44	1	0
3	C	94	0	44	1	0
3	E	94	0	44	1	0
3	G	94	0	44	1	0
4	A	1	0	0	0	0
4	C	1	0	0	1	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
5	G	1	0	0	0	0
6	A	7	0	0	0	0
6	C	7	0	0	0	0
6	E	7	0	0	0	0
6	G	7	0	0	0	0
7	B	4	0	0	0	0
7	D	4	0	0	1	0
7	F	4	0	0	0	0
7	H	4	0	0	0	0
8	A	6	0	0	0	0
8	C	2	0	0	0	0
8	E	5	0	0	0	0
8	G	2	0	0	0	0
All	All	30609	0	29156	213	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 4.

All (213) 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:E:130:TRP:HB2	1:E:135:MET:CE	1.85	1.04
1:E:130:TRP:HB2	1:E:135:MET:HE1	1.04	1.01
1:G:423:ARG:HA	1:G:693:MET:HE1	1.44	0.97
1:E:130:TRP:CB	1:E:135:MET:HE1	1.95	0.96
1:A:423:ARG:HA	1:A:693:MET:CE	1.97	0.94
1:G:423:ARG:HA	1:G:693:MET:CE	2.00	0.91
1:A:135:MET:HE1	1:A:554:CYS:O	1.70	0.90
1:G:752:ASP:OD1	1:G:785:ARG:NH1	2.09	0.85
1:C:752:ASP:OD1	1:C:785:ARG:NH1	2.10	0.84
1:C:9:ARG:NH2	2:D:45:ALA:HB1	1.94	0.82
1:A:423:ARG:HA	1:A:693:MET:HE1	1.60	0.82
1:A:256:ARG:HG3	1:A:294:THR:HG23	1.62	0.81
2:D:45:ALA:HB3	1:E:9:ARG:CZ	2.11	0.80
1:C:599:ARG:NH1	1:C:602:ASN:OD1	2.16	0.79
1:A:339:GLU:HG2	1:G:755:GLU:HA	1.65	0.79
1:A:599:ARG:NH1	1:A:602:ASN:OD1	2.16	0.78
1:E:130:TRP:HE3	1:E:135:MET:CE	1.98	0.77
1:A:843:GLN:OE1	2:B:116:ASN:ND2	2.16	0.76
1:C:423:ARG:HA	1:C:693:MET:CE	2.17	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:LEU:C	1:E:415:LEU:HD23	2.13	0.74
1:A:423:ARG:HA	1:A:693:MET:HE2	1.69	0.73
1:E:599:ARG:NH1	1:E:602:ASN:OD1	2.22	0.73
1:G:135:MET:HE1	1:G:554:CYS:O	1.90	0.71
2:D:45:ALA:HB3	1:E:9:ARG:NE	2.05	0.71
1:E:130:TRP:CB	1:E:135:MET:CE	2.63	0.71
1:E:423:ARG:HA	1:E:693:MET:CE	2.21	0.70
1:E:130:TRP:HE3	1:E:135:MET:HE2	1.58	0.68
1:C:204:TYR:HB3	1:C:463:VAL:HG11	1.76	0.68
2:D:45:ALA:CB	1:E:9:ARG:CZ	2.72	0.68
1:A:135:MET:CE	1:A:554:CYS:O	2.42	0.67
1:C:252:ILE:HD12	1:C:294:THR:HG21	1.78	0.66
1:E:130:TRP:CE3	1:E:135:MET:CE	2.79	0.66
1:E:252:ILE:HD12	1:E:294:THR:HG21	1.78	0.66
1:G:156:LYS:HE2	1:G:611:MET:HE2	1.78	0.66
1:C:423:ARG:HA	1:C:693:MET:HE1	1.77	0.65
1:E:599:ARG:HG3	1:E:599:ARG:HH11	1.61	0.65
1:C:9:ARG:HH21	2:D:45:ALA:HB1	1.61	0.64
1:E:423:ARG:HA	1:E:693:MET:HE1	1.80	0.64
1:A:256:ARG:HG3	1:A:294:THR:CG2	2.29	0.62
2:H:44:ALA:O	2:H:45:ALA:HB3	2.00	0.62
1:E:130:TRP:CE3	1:E:135:MET:HE2	2.34	0.62
1:C:561:ALA:O	1:C:566:MET:CE	2.48	0.61
1:C:423:ARG:HA	1:C:693:MET:HE2	1.82	0.61
1:G:40:ILE:O	1:G:41:ASN:OD1	2.19	0.60
1:A:204:TYR:HB3	1:A:463:VAL:HG11	1.84	0.59
1:A:40:ILE:O	1:A:41:ASN:OD1	2.20	0.59
1:G:252:ILE:HD12	1:G:294:THR:HG21	1.85	0.58
1:E:130:TRP:HE3	1:E:135:MET:HE3	1.69	0.58
1:C:832:VAL:HG22	1:C:835:LEU:HD12	1.86	0.57
1:E:561:ALA:O	1:E:566:MET:HE2	2.04	0.57
1:E:433:LEU:HD23	1:E:438:ILE:HD12	1.87	0.56
2:B:54:LEU:HD11	2:B:160:ALA:HB2	1.87	0.56
1:A:561:ALA:O	1:A:566:MET:CE	2.53	0.56
1:E:423:ARG:HA	1:E:693:MET:HE2	1.86	0.56
1:A:198:ILE:HG22	1:A:199:HIS:N	2.21	0.56
2:D:68:VAL:HG13	2:D:69:ALA:N	2.21	0.55
1:C:415:LEU:HD23	1:C:415:LEU:C	2.32	0.55
1:E:358:GLY:HA3	1:E:693:MET:HE3	1.89	0.55
1:A:413:LYS:HD2	1:A:417:TRP:NE1	2.22	0.54
1:C:135:MET:HE1	1:C:554:CYS:O	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:LYS:HD2	1:C:417:TRP:NE1	2.23	0.54
1:E:413:LYS:HD2	1:E:417:TRP:NE1	2.23	0.54
2:D:174:VAL:O	2:D:174:VAL:HG13	2.07	0.54
1:E:599:ARG:NH2	1:E:625:TRP:O	2.40	0.54
1:G:423:ARG:HA	1:G:693:MET:HE3	1.88	0.54
1:A:599:ARG:NH2	1:A:625:TRP:O	2.41	0.54
1:A:433:LEU:HD23	1:A:438:ILE:HD12	1.90	0.54
1:G:433:LEU:HD23	1:G:438:ILE:HD12	1.89	0.53
1:A:561:ALA:O	1:A:566:MET:HE3	2.08	0.53
1:G:413:LYS:HD2	1:G:417:TRP:NE1	2.23	0.52
1:A:339:GLU:HG2	1:G:755:GLU:CA	2.37	0.52
1:C:599:ARG:NH2	1:C:625:TRP:O	2.42	0.52
1:A:198:ILE:HG22	1:A:199:HIS:H	1.75	0.52
1:G:561:ALA:O	1:G:566:MET:CE	2.56	0.52
1:E:40:ILE:O	1:E:41:ASN:HB2	2.10	0.52
1:G:693:MET:HE3	1:G:695:ALA:HB2	1.92	0.51
1:G:123:ARG:HG2	1:G:545:ILE:O	2.10	0.51
1:C:28:ILE:HG21	1:C:448:LEU:O	2.11	0.51
1:C:77:VAL:HB	1:C:584:MET:HE3	1.93	0.51
1:A:255:LEU:HB3	1:A:295:ALA:HB2	1.91	0.51
1:G:123:ARG:HG2	1:G:123:ARG:HH11	1.76	0.51
1:C:123:ARG:HG2	1:C:545:ILE:O	2.10	0.51
1:A:28:ILE:HG21	1:A:448:LEU:O	2.10	0.50
1:C:561:ALA:O	1:C:566:MET:HE3	2.10	0.50
2:D:68:VAL:CG1	2:D:69:ALA:N	2.74	0.50
1:C:445:VAL:O	1:C:445:VAL:HG13	2.12	0.50
1:G:578:ARG:HD2	1:G:656:THR:O	2.12	0.50
1:G:721:ALA:HB2	1:G:791:LEU:HD13	1.93	0.50
2:H:44:ALA:O	2:H:45:ALA:CB	2.59	0.50
1:C:337:LEU:HD13	1:C:691:ARG:HH21	1.75	0.50
2:D:54:LEU:HD11	2:D:160:ALA:HB2	1.93	0.50
1:G:574:GLU:OE1	1:G:576:ARG:NH1	2.45	0.50
1:C:574:GLU:OE1	1:C:576:ARG:NH1	2.45	0.50
1:A:574:GLU:OE1	1:A:576:ARG:NH1	2.45	0.50
1:E:578:ARG:HD2	1:E:656:THR:O	2.12	0.49
2:B:70:TYR:CD1	2:B:71:PRO:HA	2.48	0.49
1:E:28:ILE:HG21	1:E:448:LEU:O	2.11	0.49
1:A:339:GLU:HG2	1:G:755:GLU:O	2.12	0.49
2:B:68:VAL:CG1	2:B:69:ALA:N	2.76	0.49
1:E:574:GLU:OE1	1:E:576:ARG:NH1	2.45	0.49
1:C:578:ARG:HD2	1:C:656:THR:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:578:ARG:CD	1:G:656:THR:O	2.61	0.49
2:H:70:TYR:CD1	2:H:71:PRO:HA	2.48	0.49
1:E:578:ARG:CD	1:E:656:THR:O	2.60	0.49
1:E:255:LEU:HB3	1:E:295:ALA:HB2	1.95	0.49
1:G:426:GLY:HA3	1:G:693:MET:HE2	1.95	0.49
1:C:135:MET:CE	1:C:554:CYS:O	2.60	0.48
1:A:578:ARG:HD2	1:A:656:THR:O	2.13	0.48
1:C:358:GLY:HA3	1:C:693:MET:HE3	1.95	0.48
1:E:337:LEU:HD13	1:E:691:ARG:HH21	1.77	0.48
2:H:54:LEU:HD11	2:H:160:ALA:HB2	1.94	0.48
1:G:832:VAL:HG22	1:G:835:LEU:HD22	1.96	0.48
1:C:255:LEU:HB3	1:C:295:ALA:HB2	1.96	0.48
1:E:721:ALA:HB2	1:E:791:LEU:HD13	1.94	0.48
1:C:578:ARG:CD	1:C:656:THR:O	2.62	0.47
1:C:742:PRO:HD2	1:C:835:LEU:HD11	1.96	0.47
1:E:293:GLN:NE2	1:E:844:SER:HB3	2.29	0.47
1:A:578:ARG:CD	1:A:656:THR:O	2.62	0.47
1:G:255:LEU:HB3	1:G:295:ALA:HB2	1.95	0.47
2:D:70:TYR:CD1	2:D:71:PRO:HA	2.48	0.47
1:C:123:ARG:HG2	1:C:123:ARG:HH11	1.77	0.47
2:D:101:THR:O	2:D:101:THR:CG2	2.63	0.47
1:A:493:THR:HG23	1:A:494:LEU:O	2.14	0.47
1:E:433:LEU:CD2	1:E:438:ILE:HD12	2.44	0.47
1:G:198:ILE:HG22	1:G:199:HIS:N	2.30	0.47
2:H:68:VAL:CG1	2:H:69:ALA:N	2.77	0.47
2:F:70:TYR:CD1	2:F:71:PRO:HA	2.49	0.47
1:C:721:ALA:HB2	1:C:791:LEU:HD13	1.95	0.47
1:C:40:ILE:O	1:C:41:ASN:HB2	2.14	0.46
1:C:693:MET:HG2	1:C:695:ALA:HB2	1.97	0.46
1:A:415:LEU:HD23	1:A:415:LEU:C	2.40	0.46
1:G:337:LEU:HD13	1:G:691:ARG:HH21	1.81	0.46
1:A:577:MET:O	1:A:578:ARG:HG3	2.16	0.46
1:C:493:THR:HG23	1:C:494:LEU:O	2.16	0.46
2:D:154:ASP:OD1	2:D:154:ASP:N	2.49	0.46
1:E:204:TYR:HB3	1:E:463:VAL:HG11	1.97	0.46
1:E:415:LEU:C	1:E:415:LEU:CD2	2.85	0.46
1:C:701:GLN:CD	1:C:701:GLN:C	2.84	0.45
1:E:130:TRP:HA	1:E:135:MET:HE2	1.98	0.45
2:F:54:LEU:HD11	2:F:160:ALA:HB2	1.97	0.45
2:H:154:ASP:OD1	2:H:154:ASP:N	2.49	0.45
1:G:28:ILE:HG21	1:G:448:LEU:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:TYR:O	1:E:500:LYS:HE2	2.16	0.45
1:A:169:ASP:OD1	1:A:169:ASP:C	2.59	0.45
1:C:740:ARG:O	1:C:835:LEU:HD22	2.16	0.45
1:C:76:VAL:HG23	1:C:117:ARG:HD2	1.99	0.45
1:C:490:TYR:O	1:C:500:LYS:HE2	2.17	0.45
1:G:198:ILE:HG22	1:G:199:HIS:H	1.82	0.45
1:C:293:GLN:NE2	1:C:844:SER:HB2	2.32	0.44
1:E:130:TRP:CE3	1:E:135:MET:HE3	2.47	0.44
1:G:415:LEU:C	1:G:415:LEU:HD23	2.42	0.44
2:D:101:THR:O	2:D:101:THR:HG23	2.18	0.44
2:H:101:THR:O	2:H:101:THR:CG2	2.66	0.44
1:C:240:LEU:HD23	1:C:286:VAL:HG23	1.99	0.44
1:G:490:TYR:O	1:G:500:LYS:HE2	2.17	0.44
1:G:135:MET:CE	1:G:554:CYS:O	2.64	0.44
1:G:169:ASP:C	1:G:169:ASP:OD1	2.61	0.44
1:A:490:TYR:O	1:A:500:LYS:HE2	2.18	0.44
1:A:445:VAL:O	1:A:445:VAL:HG13	2.18	0.43
1:E:577:MET:O	1:E:578:ARG:HG3	2.18	0.43
1:G:40:ILE:O	1:G:41:ASN:CG	2.62	0.43
1:G:693:MET:HG2	1:G:695:ALA:HB2	2.01	0.43
1:C:577:MET:O	1:C:578:ARG:HG3	2.18	0.43
1:E:169:ASP:OD1	1:E:169:ASP:C	2.62	0.43
1:A:693:MET:HG2	1:A:695:ALA:HB2	2.00	0.43
1:C:235:VAL:O	1:C:411:TYR:HA	2.19	0.43
2:D:45:ALA:CB	1:E:9:ARG:NH2	2.81	0.43
1:A:413:LYS:HD2	1:A:417:TRP:CE2	2.54	0.43
2:H:54:LEU:HD13	2:H:68:VAL:HG11	2.00	0.43
1:E:493:THR:HG23	1:E:494:LEU:O	2.19	0.43
1:C:9:ARG:NE	2:F:45:ALA:HA	2.34	0.43
1:C:740:ARG:O	1:C:835:LEU:CD2	2.66	0.43
1:C:200:ASN:ND2	4:C:2003:O:O	2.50	0.42
1:G:577:MET:O	1:G:578:ARG:HG3	2.18	0.42
1:G:204:TYR:HB3	1:G:463:VAL:HG11	2.00	0.42
1:A:235:VAL:O	1:A:411:TYR:HA	2.20	0.42
1:E:130:TRP:CA	1:E:135:MET:CE	2.98	0.42
1:E:235:VAL:O	1:E:411:TYR:HA	2.19	0.42
1:G:423:ARG:CA	1:G:693:MET:HE1	2.32	0.42
1:C:450:GLY:HA2	3:C:2002:MGD:H11	2.01	0.42
1:G:433:LEU:CD2	1:G:438:ILE:HD12	2.49	0.42
1:A:174:GLY:HA2	3:A:2001:MGD:C6	2.49	0.42
2:B:154:ASP:N	2:B:154:ASP:OD1	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:693:MET:HG2	1:E:695:ALA:HB2	2.01	0.42
1:E:445:VAL:HG13	1:E:445:VAL:O	2.20	0.42
1:E:8:ASP:HB3	2:F:47:VAL:HG21	2.01	0.42
1:G:311:LEU:CD1	1:G:427:ALA:HB2	2.49	0.42
1:A:122:GLN:O	1:A:547:PRO:HD3	2.20	0.42
1:C:413:LYS:HD2	1:C:417:TRP:CE2	2.55	0.42
1:G:174:GLY:HA2	3:G:2001:MGD:C6	2.50	0.42
1:E:174:GLY:HA2	3:E:2001:MGD:C6	2.50	0.41
1:A:208:VAL:HB	1:A:211:THR:HG22	2.02	0.41
1:C:169:ASP:OD1	1:C:169:ASP:C	2.62	0.41
1:A:339:GLU:CG	1:G:755:GLU:O	2.69	0.41
1:E:514:MET:HE3	1:E:529:ILE:HD11	2.03	0.41
1:A:40:ILE:O	1:A:41:ASN:CG	2.64	0.41
1:G:235:VAL:O	1:G:411:TYR:HA	2.20	0.41
1:C:198:ILE:HG22	1:C:199:HIS:N	2.36	0.41
1:G:413:LYS:HD2	1:G:417:TRP:CE2	2.56	0.41
1:A:752:ASP:OD1	1:A:785:ARG:HG3	2.20	0.41
1:A:701:GLN:C	1:A:701:GLN:CD	2.89	0.41
2:F:101:THR:O	2:F:101:THR:CG2	2.69	0.41
1:A:198:ILE:CG2	1:A:199:HIS:N	2.84	0.41
1:A:269:GLU:OE1	1:E:823:ARG:NH1	2.54	0.41
1:A:721:ALA:HB2	1:A:791:LEU:HD13	2.03	0.41
2:D:106:LYS:HB2	7:D:2006:FES:S2	2.61	0.41
1:E:122:GLN:O	1:E:547:PRO:HD3	2.21	0.40
1:E:654:MET:HE2	1:E:654:MET:HB3	1.94	0.40
1:C:723:VAL:HG23	1:C:724:VAL:HG23	2.03	0.40
1:E:423:ARG:HG2	1:E:693:MET:CE	2.51	0.40
1:E:651:LEU:HD23	1:E:651:LEU:HA	1.94	0.40
1:E:490:TYR:O	1:E:500:LYS:CE	2.70	0.40
1:E:701:GLN:CD	1:E:701:GLN:C	2.89	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:C:686:ASP:O	1:C:686:ASP:O[2_545]	1.73	0.47

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	841/845 (100%)	810 (96%)	30 (4%)	1 (0%)	48	73
1	C	842/845 (100%)	812 (96%)	29 (3%)	1 (0%)	48	73
1	E	841/845 (100%)	815 (97%)	25 (3%)	1 (0%)	48	73
1	G	841/845 (100%)	809 (96%)	31 (4%)	1 (0%)	48	73
2	B	130/175 (74%)	125 (96%)	5 (4%)	0	100	100
2	D	130/175 (74%)	126 (97%)	4 (3%)	0	100	100
2	F	130/175 (74%)	121 (93%)	7 (5%)	2 (2%)	8	22
2	H	130/175 (74%)	125 (96%)	4 (3%)	1 (1%)	16	37
All	All	3885/4080 (95%)	3743 (96%)	135 (4%)	7 (0%)	43	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	154	ASP
2	H	45	ALA
2	F	155	ASN
1	E	811	ILE
1	A	811	ILE
1	G	811	ILE
1	C	811	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	677/678 (100%)	661 (98%)	16 (2%)	43	72
1	C	678/678 (100%)	658 (97%)	20 (3%)	37	67
1	E	677/678 (100%)	659 (97%)	18 (3%)	39	69
1	G	677/678 (100%)	658 (97%)	19 (3%)	38	68
2	B	105/130 (81%)	103 (98%)	2 (2%)	50	77
2	D	105/130 (81%)	101 (96%)	4 (4%)	29	58
2	F	105/130 (81%)	103 (98%)	2 (2%)	50	77
2	H	105/130 (81%)	100 (95%)	5 (5%)	23	50
All	All	3129/3232 (97%)	3043 (97%)	86 (3%)	39	69

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	CYS
1	A	46	THR
1	A	49	GLN
1	A	89	LYS
1	A	134	GLN
1	A	329	ARG
1	A	347	TYR
1	A	440	ARG
1	A	463	VAL
1	A	599	ARG
1	A	701	GLN
1	A	733	GLU
1	A	785	ARG
1	A	792	PHE
1	A	799	GLN
1	A	832	VAL
2	B	68	VAL
2	B	101	THR
1	C	27	CYS
1	C	46	THR
1	C	49	GLN
1	C	89	LYS
1	C	121[A]	GLN
1	C	121[B]	GLN
1	C	123	ARG
1	C	329	ARG
1	C	347	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	440	ARG
1	C	522	ARG
1	C	599	ARG
1	C	691	ARG
1	C	701	GLN
1	C	733	GLU
1	C	785	ARG
1	C	792	PHE
1	C	799	GLN
1	C	832	VAL
1	C	843	GLN
2	D	68	VAL
2	D	101	THR
2	D	102	ILE
2	D	154	ASP
1	E	27	CYS
1	E	46	THR
1	E	49	GLN
1	E	89	LYS
1	E	134	GLN
1	E	329	ARG
1	E	346	LEU
1	E	347	TYR
1	E	440	ARG
1	E	463	VAL
1	E	522	ARG
1	E	599	ARG
1	E	691	ARG
1	E	701	GLN
1	E	733	GLU
1	E	792	PHE
1	E	799	GLN
1	E	832	VAL
2	F	101	THR
2	F	154	ASP
1	G	27	CYS
1	G	46	THR
1	G	49	GLN
1	G	89	LYS
1	G	123	ARG
1	G	134	GLN
1	G	329	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	347	TYR
1	G	440	ARG
1	G	463	VAL
1	G	522	ARG
1	G	691	ARG
1	G	701	GLN
1	G	708	GLN
1	G	785	ARG
1	G	792	PHE
1	G	799	GLN
1	G	832	VAL
1	G	843	GLN
2	H	68	VAL
2	H	78	VAL
2	H	84	THR
2	H	101	THR
2	H	154	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	21	ASN
1	A	134	GLN
1	A	220	ASN
1	A	478	GLN
1	A	619	GLN
1	A	637	ASN
1	C	21	ASN
1	C	61	GLN
1	C	134	GLN
1	C	220	ASN
1	C	293	GLN
2	D	120	ASN
2	D	143	GLN
1	E	21	ASN
1	E	79	GLN
1	E	220	ASN
1	E	293	GLN
1	E	478	GLN
1	E	527	ASN
1	E	535	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	542	ASN
1	E	619	GLN
2	F	143	GLN
1	G	6	HIS
1	G	21	ASN
1	G	79	GLN
1	G	220	ASN
1	G	527	ASN
1	G	535	GLN
1	G	637	ASN
2	H	116	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
6	F3S	C	2005	1	0,9,9	-	-	-		
7	FES	D	2006	2	0,4,4	-	-	-		
3	MGD	E	2001	5	45,52,52	1.39	7 (15%)	54,81,81	1.90	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MGD	C	2002	5	45,52,52	1.44	8 (17%)	54,81,81	1.83	11 (20%)
6	F3S	G	2005	1	0,9,9	-	-	-		
7	FES	F	2006	2	0,4,4	-	-	-		
3	MGD	A	2001	5	45,52,52	1.29	5 (11%)	54,81,81	1.80	14 (25%)
3	MGD	C	2001	5	45,52,52	1.36	6 (13%)	54,81,81	1.83	14 (25%)
6	F3S	E	2005	1	0,9,9	-	-	-		
7	FES	B	2006	2	0,4,4	-	-	-		
3	MGD	G	2001	5	45,52,52	1.36	5 (11%)	54,81,81	1.96	14 (25%)
3	MGD	A	2002	5	45,52,52	1.38	5 (11%)	54,81,81	2.05	13 (24%)
6	F3S	A	2005	1	0,9,9	-	-	-		
3	MGD	E	2002	5	45,52,52	1.38	8 (17%)	54,81,81	2.20	12 (22%)
3	MGD	G	2002	5	45,52,52	1.41	6 (13%)	54,81,81	2.10	15 (27%)
7	FES	H	2006	2	0,4,4	-	-	-		

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
6	F3S	C	2005	1	-	-	0/3/3/3
7	FES	D	2006	2	-	-	0/1/1/1
3	MGD	E	2001	5	-	5/22/66/66	0/6/6/6
3	MGD	C	2002	5	-	3/22/66/66	0/6/6/6
6	F3S	G	2005	1	-	-	0/3/3/3
7	FES	F	2006	2	-	-	0/1/1/1
3	MGD	A	2001	5	-	4/22/66/66	0/6/6/6
3	MGD	C	2001	5	-	4/22/66/66	0/6/6/6
6	F3S	E	2005	1	-	-	0/3/3/3
7	FES	B	2006	2	-	-	0/1/1/1
3	MGD	G	2001	5	-	5/22/66/66	0/6/6/6
3	MGD	A	2002	5	-	3/22/66/66	0/6/6/6
6	F3S	A	2005	1	-	-	0/3/3/3
3	MGD	E	2002	5	-	2/22/66/66	0/6/6/6
3	MGD	G	2002	5	-	3/22/66/66	0/6/6/6
7	FES	H	2006	2	-	-	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2002	MGD	C16-C21	5.87	1.48	1.38
3	C	2002	MGD	C16-C21	5.17	1.47	1.38
3	E	2001	MGD	C16-C21	5.07	1.47	1.38
3	G	2001	MGD	C16-C21	5.02	1.47	1.38
3	C	2001	MGD	C16-C21	4.91	1.47	1.38
3	A	2002	MGD	C16-C21	4.84	1.46	1.38
3	A	2001	MGD	C16-C21	3.93	1.45	1.38
3	E	2002	MGD	C16-C21	3.89	1.45	1.38
3	A	2001	MGD	C17-N18	-3.33	1.32	1.38
3	C	2002	MGD	C5-C4	3.33	1.48	1.38
3	G	2001	MGD	C5-N7	-3.02	1.33	1.39
3	E	2002	MGD	C5-C4	2.91	1.46	1.38
3	G	2002	MGD	C5-C4	2.90	1.46	1.38
3	E	2001	MGD	C5-N7	-2.85	1.33	1.39
3	E	2001	MGD	C6-N1	-2.78	1.33	1.38
3	C	2001	MGD	C5-N7	-2.73	1.33	1.39
3	A	2002	MGD	C5-N7	-2.72	1.33	1.39
3	A	2002	MGD	C17-N18	-2.69	1.33	1.38
3	A	2001	MGD	C4-N9	-2.67	1.31	1.38
3	C	2001	MGD	C4-N9	-2.66	1.31	1.38
3	E	2002	MGD	C17-N18	-2.63	1.34	1.38
3	A	2001	MGD	C5-C4	2.62	1.46	1.38
3	G	2002	MGD	C6-N1	-2.61	1.34	1.38
3	G	2002	MGD	C5-N7	-2.61	1.34	1.39
3	C	2001	MGD	C17-N18	-2.60	1.34	1.38
3	E	2002	MGD	C6-N1	-2.56	1.34	1.38
3	E	2002	MGD	C5-N7	-2.54	1.34	1.39
3	G	2001	MGD	C5-C4	2.50	1.45	1.38
3	A	2002	MGD	C5-C4	2.45	1.45	1.38
3	C	2001	MGD	C6-N1	-2.44	1.34	1.38
3	E	2002	MGD	O11-C11	-2.41	1.40	1.43
3	G	2002	MGD	C17-N18	-2.38	1.34	1.38
3	C	2001	MGD	C5-C4	2.33	1.45	1.38
3	E	2001	MGD	C16-C17	2.33	1.48	1.42
3	E	2001	MGD	C4-N9	-2.31	1.32	1.38
3	C	2002	MGD	C16-C17	2.25	1.48	1.42
3	C	2002	MGD	C21-N22	-2.25	1.33	1.35
3	A	2002	MGD	O11-C11	-2.25	1.40	1.43
3	G	2002	MGD	C16-C17	2.23	1.48	1.42
3	E	2001	MGD	C17-N18	-2.22	1.34	1.38
3	E	2002	MGD	C4-N9	-2.20	1.32	1.38
3	C	2002	MGD	C17-N18	-2.19	1.34	1.38
3	E	2001	MGD	C5-C4	2.19	1.44	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2001	MGD	C21-N22	-2.18	1.33	1.35
3	E	2002	MGD	C21-N22	-2.11	1.33	1.35
3	A	2001	MGD	C5-N7	-2.11	1.35	1.39
3	G	2001	MGD	C4-N9	-2.10	1.32	1.38
3	C	2002	MGD	C6-N1	-2.06	1.35	1.38
3	C	2002	MGD	O11-C11	-2.05	1.41	1.43
3	C	2002	MGD	C5-N7	-2.04	1.35	1.39

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2002	MGD	O11-C23-N22	-7.45	100.91	108.57
3	G	2002	MGD	O11-C23-N22	-6.08	102.32	108.57
3	A	2002	MGD	O11-C23-C14	5.86	112.87	108.96
3	A	2002	MGD	C5-C4-N3	-5.85	118.97	128.46
3	E	2002	MGD	C5-C4-N3	-5.79	119.07	128.46
3	G	2002	MGD	C5-C4-N3	-5.55	119.45	128.46
3	C	2002	MGD	O11-C23-N22	-5.45	102.97	108.57
3	E	2001	MGD	C5-C4-N3	-5.12	120.15	128.46
3	C	2001	MGD	C19-N20-C21	5.00	122.45	113.43
3	G	2001	MGD	C5-C4-N3	-4.98	120.39	128.46
3	C	2002	MGD	C5-C4-N3	-4.83	120.63	128.46
3	C	2001	MGD	C5-C4-N3	-4.75	120.75	128.46
3	G	2001	MGD	C2-N3-C4	4.70	120.68	112.30
3	E	2002	MGD	C19-N20-C21	4.62	121.76	113.43
3	A	2001	MGD	C19-N20-C21	4.58	121.70	113.43
3	G	2002	MGD	C2-N3-C4	4.55	120.40	112.30
3	E	2002	MGD	O11-C23-C14	4.52	111.98	108.96
3	G	2002	MGD	N9-C4-N3	4.49	134.95	125.94
3	A	2001	MGD	C5-C4-N3	-4.47	121.21	128.46
3	E	2001	MGD	N9-C4-N3	4.47	134.91	125.94
3	A	2002	MGD	C2-N3-C4	4.40	120.15	112.30
3	G	2002	MGD	C19-N20-C21	4.33	121.24	113.43
3	E	2002	MGD	C2-N3-C4	4.31	119.98	112.30
3	C	2002	MGD	C19-N20-C21	4.30	121.19	113.43
3	C	2002	MGD	N9-C4-N3	4.28	134.54	125.94
3	C	2001	MGD	C2-N3-C4	4.23	119.83	112.30
3	A	2002	MGD	C19-N20-C21	4.13	120.89	113.43
3	A	2001	MGD	C2-N3-C4	4.12	119.64	112.30
3	G	2001	MGD	C19-N20-C21	4.11	120.84	113.43
3	E	2001	MGD	C2-N3-C4	4.07	119.55	112.30
3	E	2001	MGD	C19-N20-C21	4.05	120.74	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	MGD	N9-C4-N3	4.00	133.98	125.94
3	G	2002	MGD	C4'-O4'-C1'	-3.85	100.98	109.47
3	E	2002	MGD	N9-C4-N3	3.74	133.44	125.94
3	E	2001	MGD	O6-C6-C5	-3.72	116.74	126.60
3	G	2001	MGD	PA-O3B-PB	-3.60	120.47	132.83
3	C	2002	MGD	C4'-O4'-C1'	-3.59	101.55	109.47
3	E	2002	MGD	O17-C17-C16	-3.59	119.01	127.24
3	G	2001	MGD	N9-C4-N3	3.53	133.03	125.94
3	G	2001	MGD	O6-C6-C5	-3.50	117.32	126.60
3	G	2001	MGD	O17-C17-C16	-3.43	119.39	127.24
3	C	2001	MGD	N9-C4-N3	3.40	132.76	125.94
3	A	2001	MGD	N9-C4-N3	3.31	132.59	125.94
3	G	2001	MGD	C6-C5-N7	3.28	136.34	130.25
3	A	2001	MGD	C6-C5-N7	3.27	136.33	130.25
3	A	2002	MGD	C4-C5-N7	-3.26	105.56	110.72
3	C	2002	MGD	C2-N3-C4	3.24	118.07	112.30
3	A	2002	MGD	O11-C23-N22	-3.24	105.24	108.57
3	C	2001	MGD	C6-C5-N7	3.22	136.23	130.25
3	C	2002	MGD	O17-C17-C16	-3.13	120.06	127.24
3	G	2002	MGD	O11-C23-C14	3.12	111.04	108.96
3	A	2001	MGD	PA-O3B-PB	-3.12	122.13	132.83
3	E	2002	MGD	C4'-O4'-C1'	-3.07	102.69	109.47
3	G	2002	MGD	O17-C17-C16	-3.05	120.25	127.24
3	A	2002	MGD	C6-C5-N7	3.04	135.90	130.25
3	E	2002	MGD	C6-C5-N7	3.00	135.83	130.25
3	A	2002	MGD	C4'-O4'-C1'	-2.99	102.88	109.47
3	G	2002	MGD	O4'-C1'-N9	2.92	115.04	108.36
3	G	2002	MGD	C6-C5-N7	2.92	135.67	130.25
3	E	2002	MGD	C4-C5-N7	-2.89	106.15	110.72
3	G	2001	MGD	N2-C2-N1	2.80	122.68	116.71
3	G	2001	MGD	N2-C2-N3	-2.78	114.31	119.73
3	C	2001	MGD	PA-O3B-PB	-2.78	123.27	132.83
3	A	2001	MGD	O17-C17-C16	-2.78	120.86	127.24
3	E	2001	MGD	O17-C17-C16	-2.74	120.97	127.24
3	A	2001	MGD	O6-C6-C5	-2.68	119.49	126.60
3	E	2001	MGD	O11-C23-N22	2.64	111.28	108.57
3	A	2002	MGD	O17-C17-C16	-2.62	121.24	127.24
3	C	2001	MGD	C4-C5-N7	-2.61	106.59	110.72
3	E	2001	MGD	PA-O3B-PB	-2.58	123.99	132.83
3	E	2001	MGD	C6-C5-N7	2.55	135.00	130.25
3	C	2002	MGD	C6-C5-N7	2.49	134.88	130.25
3	C	2001	MGD	O17-C17-C16	-2.48	121.55	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2002	MGD	C8-N7-C5	2.48	108.72	104.24
3	E	2001	MGD	O4'-C4'-C3'	2.44	109.94	105.11
3	A	2001	MGD	C19-N18-C17	-2.42	120.68	125.10
3	C	2001	MGD	O6-C6-C5	-2.40	120.25	126.60
3	E	2001	MGD	O6-C6-N1	2.39	124.70	120.12
3	A	2001	MGD	C1'-N9-C4	-2.37	119.48	126.50
3	E	2002	MGD	C16-C17-N18	2.35	119.31	112.31
3	G	2001	MGD	O6-C6-N1	2.32	124.57	120.12
3	G	2002	MGD	C16-C17-N18	2.31	119.18	112.31
3	A	2001	MGD	C16-C17-N18	2.30	119.15	112.31
3	G	2001	MGD	C4-C5-N7	-2.29	107.09	110.72
3	G	2002	MGD	O6-C6-C5	-2.29	120.53	126.60
3	G	2002	MGD	C17-C16-N15	2.22	122.71	116.76
3	A	2001	MGD	C17-C16-N15	2.19	122.63	116.76
3	C	2001	MGD	C1'-N9-C4	-2.18	120.03	126.50
3	C	2001	MGD	C17-C16-N15	2.17	122.58	116.76
3	G	2002	MGD	C5-C6-N1	2.12	118.57	113.19
3	G	2001	MGD	C2-N1-C6	-2.11	121.24	125.10
3	E	2001	MGD	C5-C6-N1	2.11	118.56	113.19
3	E	2002	MGD	O2A-PA-O1A	2.10	122.64	112.24
3	C	2002	MGD	C4-C5-N7	-2.10	107.40	110.72
3	C	2001	MGD	O2B-PB-O1B	2.09	122.56	112.24
3	G	2002	MGD	C4-C5-N7	-2.09	107.42	110.72
3	C	2002	MGD	C8-N9-C4	2.08	110.00	106.05
3	C	2002	MGD	C17-C16-N15	2.07	122.31	116.76
3	A	2002	MGD	C2-N1-C6	-2.05	121.36	125.10
3	G	2001	MGD	O2A-PA-O1A	2.05	122.38	112.24
3	A	2001	MGD	C4-C5-N7	-2.04	107.50	110.72
3	A	2002	MGD	O6-C6-C5	-2.03	121.21	126.60
3	A	2001	MGD	O2A-PA-O1A	2.02	122.21	112.24
3	C	2001	MGD	N19-C19-N18	2.01	120.99	116.71
3	C	2001	MGD	O4'-C4'-C3'	2.00	109.08	105.11

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2001	MGD	C5'-O5'-PB-O3B
3	A	2002	MGD	PA-O3B-PB-O5'
3	A	2002	MGD	C5'-O5'-PB-O1B
3	A	2002	MGD	C5'-O5'-PB-O3B
3	C	2001	MGD	PA-O3B-PB-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	2001	MGD	C5'-O5'-PB-O3B
3	E	2001	MGD	C5'-O5'-PB-O3B
3	G	2001	MGD	PA-O3B-PB-O5'
3	G	2001	MGD	C5'-O5'-PB-O1B
3	G	2001	MGD	C5'-O5'-PB-O3B
3	G	2002	MGD	PA-O3B-PB-O5'
3	G	2002	MGD	C5'-O5'-PB-O1B
3	G	2002	MGD	C5'-O5'-PB-O3B
3	G	2001	MGD	O4'-C4'-C5'-O5'
3	A	2001	MGD	PA-O3B-PB-O5'
3	C	2002	MGD	PA-O3B-PB-O5'
3	E	2001	MGD	PA-O3B-PB-O5'
3	E	2002	MGD	PA-O3B-PB-O5'
3	E	2001	MGD	O4'-C4'-C5'-O5'
3	C	2002	MGD	C5'-O5'-PB-O3B
3	A	2001	MGD	C5'-O5'-PB-O1B
3	C	2001	MGD	C5'-O5'-PB-O1B
3	E	2001	MGD	C5'-O5'-PB-O1B
3	A	2001	MGD	O4'-C4'-C5'-O5'
3	G	2001	MGD	C3'-C4'-C5'-O5'
3	C	2001	MGD	O4'-C4'-C5'-O5'
3	C	2002	MGD	C5'-O5'-PB-O1B
3	E	2002	MGD	C5'-O5'-PB-O1B
3	E	2001	MGD	C3'-C4'-C5'-O5'

There are no ring outliers.

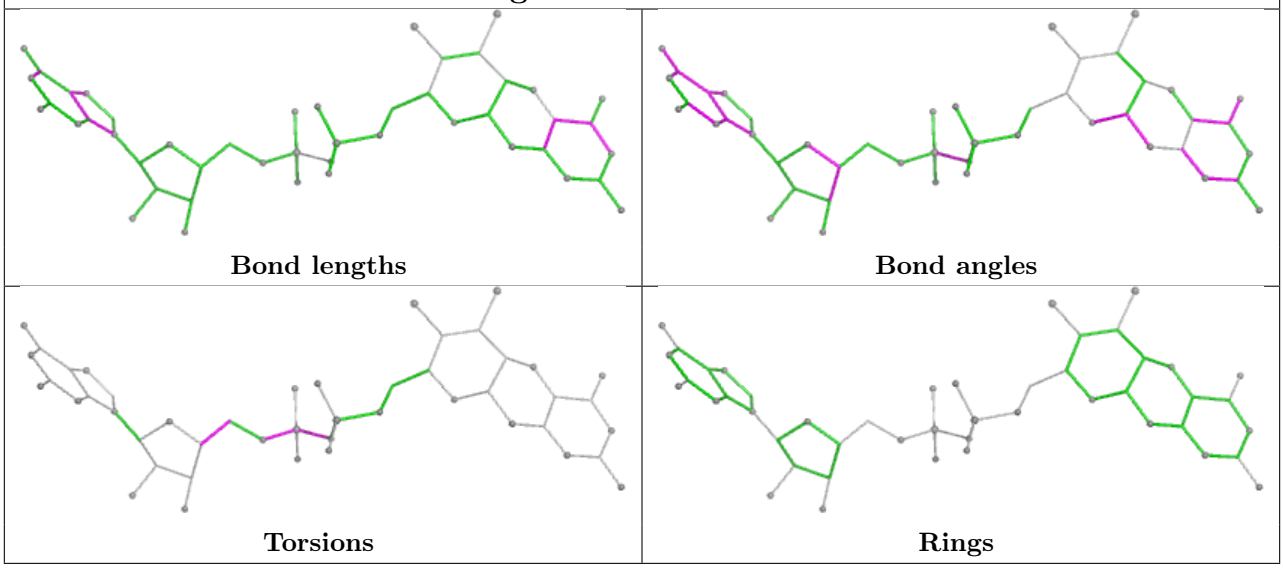
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2006	FES	1	0
3	E	2001	MGD	1	0
3	C	2002	MGD	1	0
3	A	2001	MGD	1	0
3	G	2001	MGD	1	0

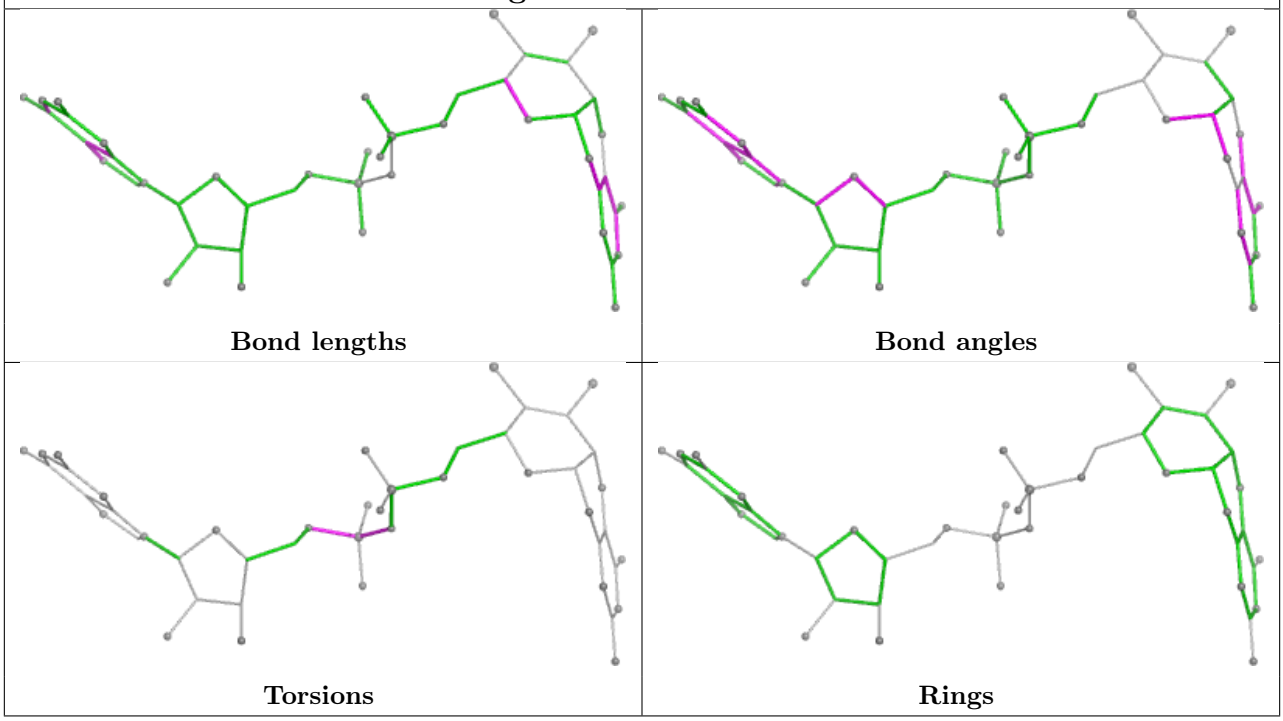
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

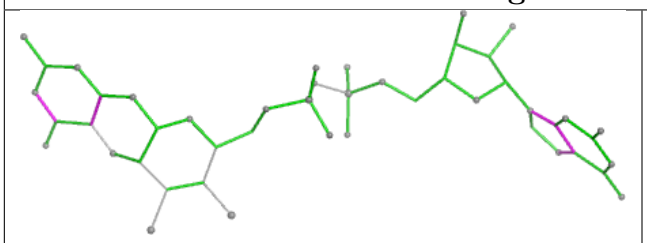
Ligand MGD E 2001



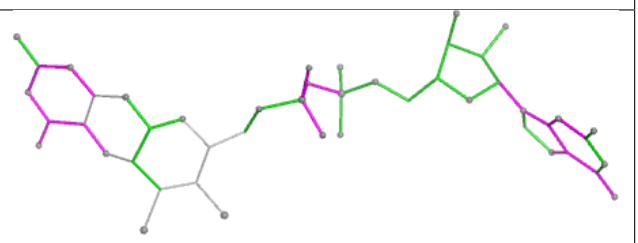
Ligand MGD C 2002



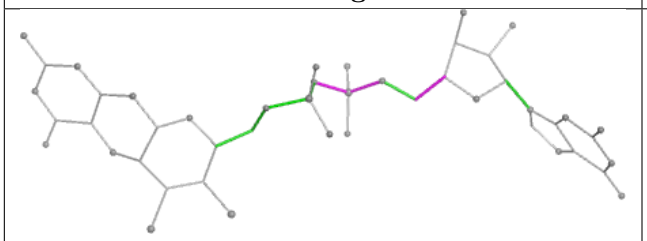
Ligand MGD A 2001



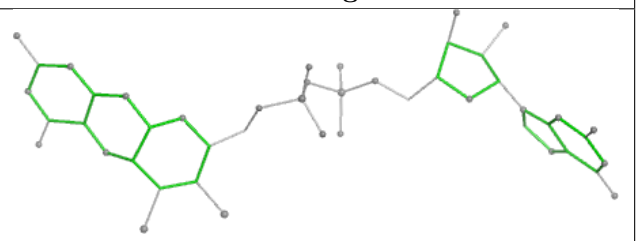
Bond lengths



Bond angles

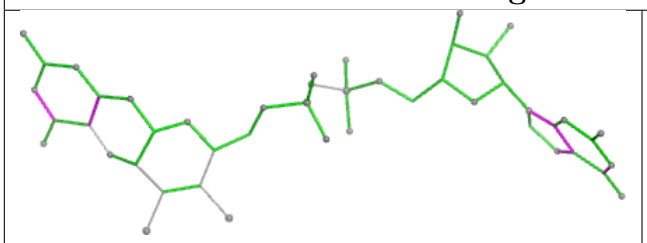


Torsions

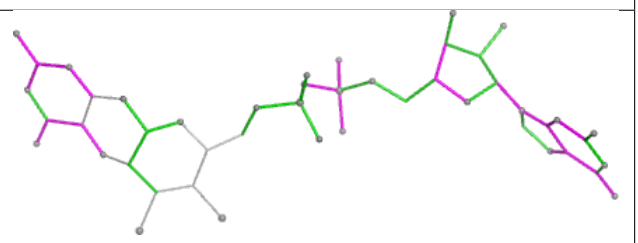


Rings

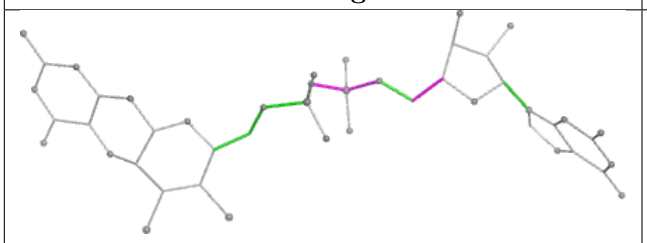
Ligand MGD C 2001



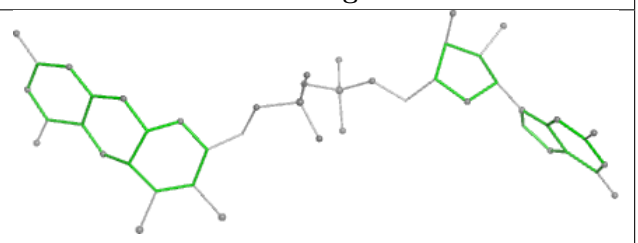
Bond lengths



Bond angles

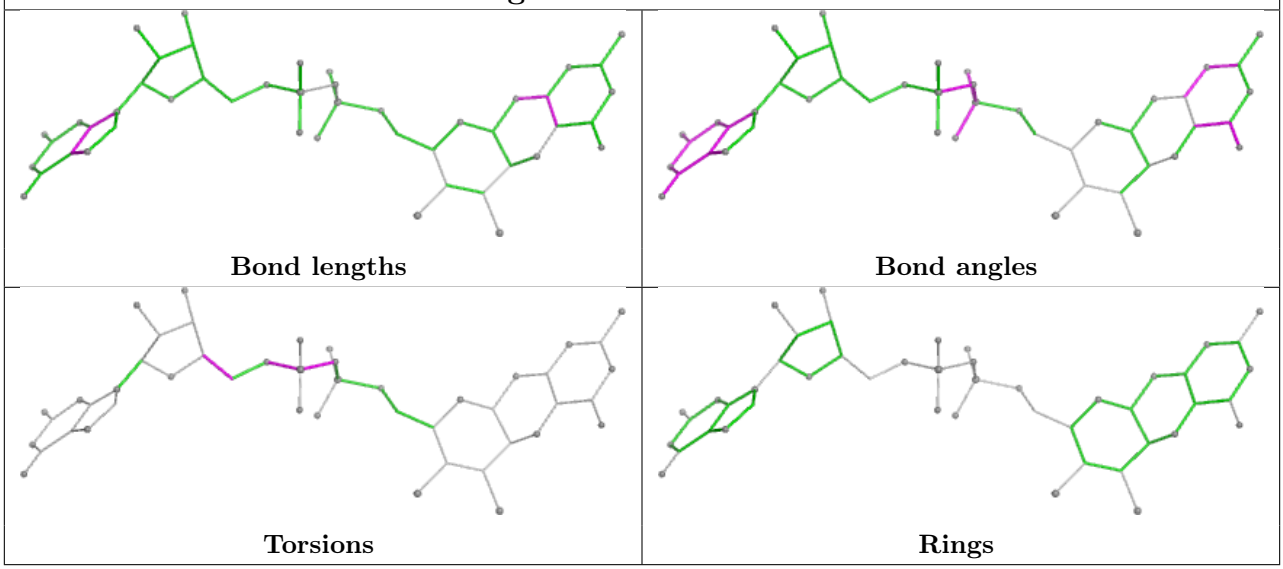


Torsions

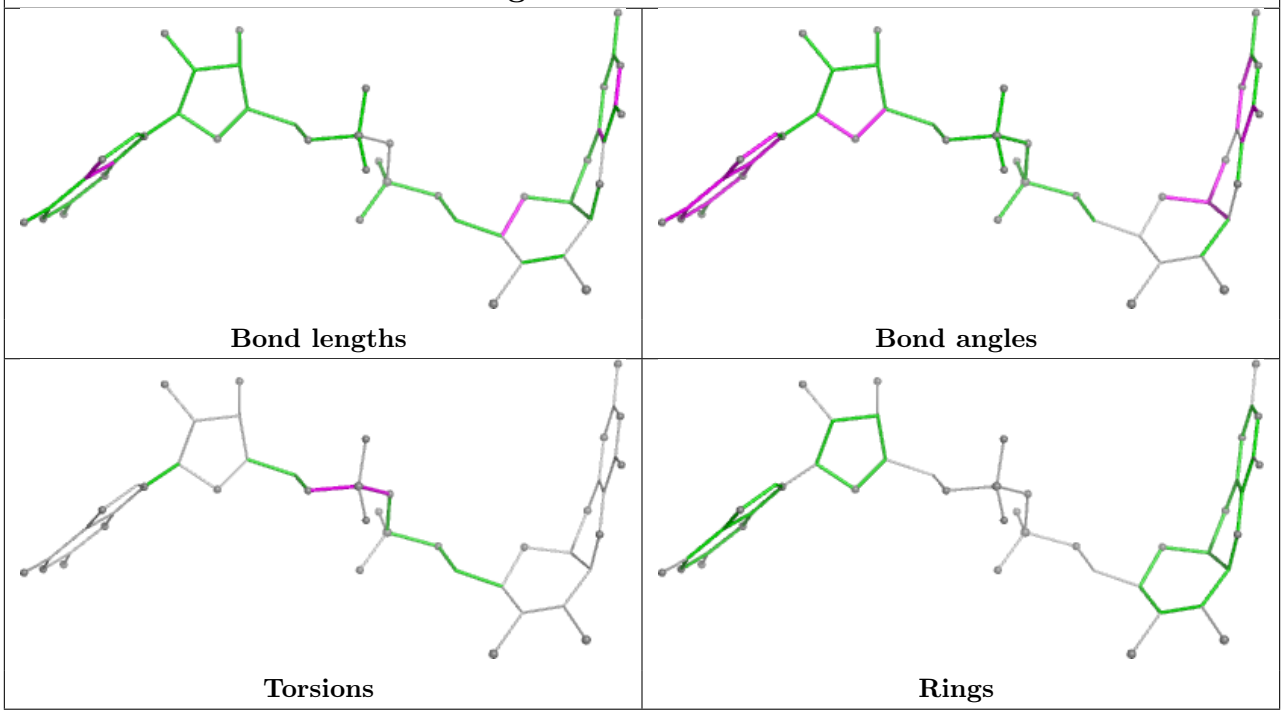


Rings

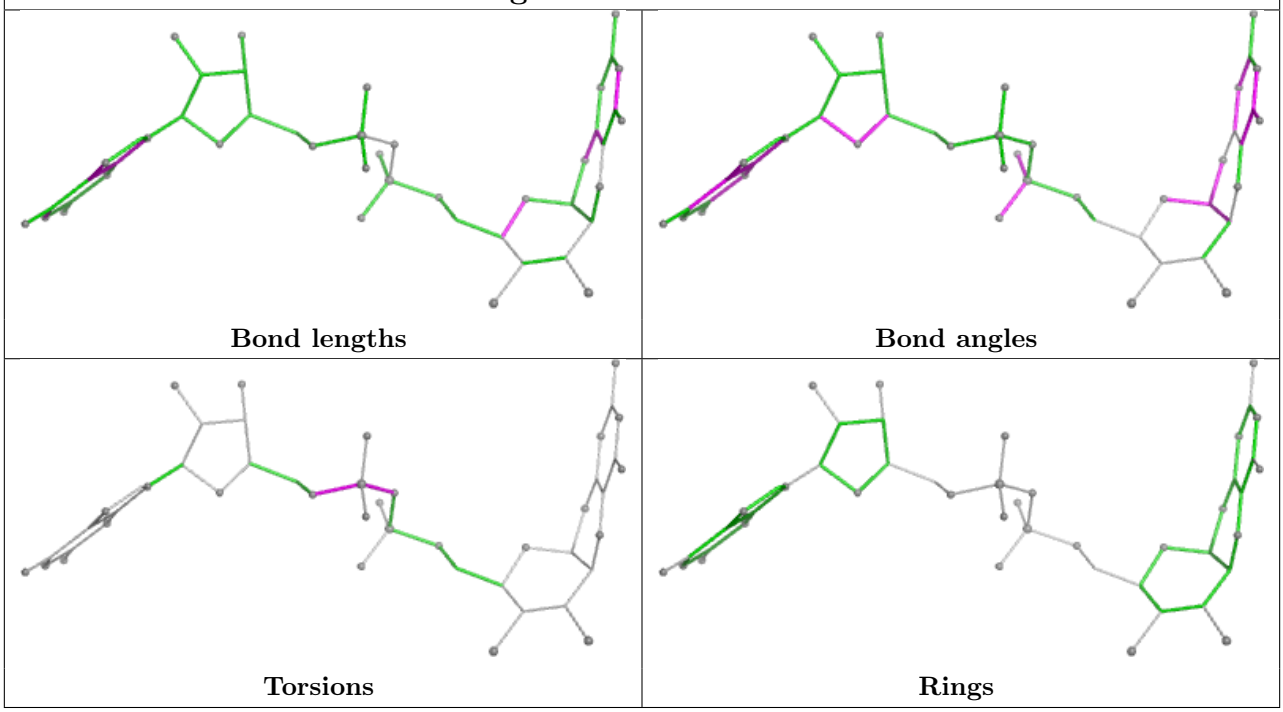
Ligand MGD G 2001



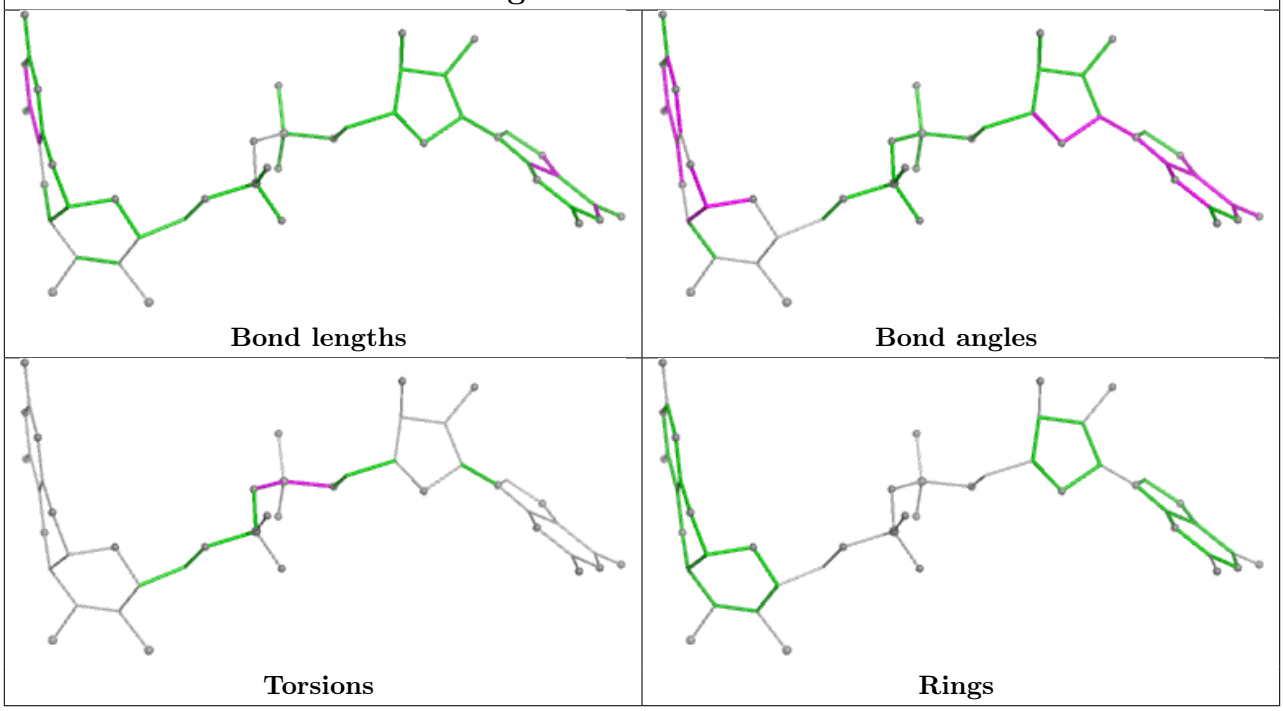
Ligand MGD A 2002



Ligand MGD E 2002



Ligand MGD G 2002



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	843/845 (99%)	0.24	29 (3%)	48	44	44, 49, 70, 93	0
1	C	843/845 (99%)	0.29	32 (3%)	44	40	32, 49, 72, 104	1 (0%)
1	E	843/845 (99%)	0.35	33 (3%)	43	39	45, 51, 77, 105	0
1	G	843/845 (99%)	0.41	36 (4%)	40	36	44, 53, 83, 112	0
2	B	132/175 (75%)	0.95	16 (12%)	8	7	49, 69, 105, 133	0
2	D	132/175 (75%)	2.20	34 (25%)	1	1	47, 68, 240, 343	0
2	F	132/175 (75%)	0.94	14 (10%)	11	9	49, 69, 96, 105	0
2	H	132/175 (75%)	1.72	35 (26%)	1	1	49, 78, 168, 322	0
All	All	3900/4080 (95%)	0.48	229 (5%)	28	25	32, 52, 85, 343	1 (0%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	45	ALA	14.3
2	D	46	GLY	13.6
2	H	45	ALA	11.0
2	H	46	GLY	10.8
2	D	164	ASP	10.7
2	D	47	VAL	10.6
2	D	49	TYR	10.4
2	D	48	GLU	9.7
2	D	165	GLU	9.5
2	H	47	VAL	9.4
2	D	54	LEU	9.2
2	H	162	GLY	8.7
2	D	55	ALA	8.6
2	D	159	PHE	8.6
2	D	155	ASN	8.4
2	H	48	GLU	8.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	51	ALA	8.3
2	D	158	ILE	8.1
2	H	161	GLU	7.8
2	H	49	TYR	7.7
2	D	56	ASN	7.4
2	D	153	ALA	7.0
2	D	160	ALA	6.8
2	D	163	VAL	6.7
2	D	157	ASP	6.6
2	D	161	GLU	6.5
2	D	156	GLY	6.3
2	D	162	GLY	6.3
1	A	269	GLU	6.0
2	H	160	ALA	6.0
1	E	41	ASN	6.0
2	D	50	PRO	5.9
2	D	154	ASP	5.8
2	H	51	ALA	5.7
2	D	52	ASN	5.6
2	B	45	ALA	5.5
1	E	340	GLY	5.4
1	G	401	GLY	5.2
1	G	273	GLU	5.1
2	H	44	ALA	5.1
2	F	44	ALA	5.0
2	D	53	ARG	5.0
1	E	269	GLU	4.8
1	G	269	GLU	4.7
1	C	41	ASN	4.7
2	H	154	ASP	4.7
1	C	269	GLU	4.5
1	E	265	GLU	4.3
2	D	44	ALA	4.2
2	B	51	ALA	4.1
2	H	155	ASN	4.1
2	H	50	PRO	4.0
1	A	339	GLU	4.0
2	D	174	VAL	3.9
1	A	844	SER	3.9
1	E	400	GLU	3.9
1	E	339	GLU	3.8
1	E	523	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	154	ASP	3.8
2	B	49	TYR	3.8
2	H	158	ILE	3.8
1	G	843	GLN	3.7
1	G	49	GLN	3.7
1	E	686	ASP	3.7
1	G	400	GLU	3.6
1	G	686	ASP	3.6
2	H	92	PRO	3.6
1	E	624	ASP	3.6
1	A	340	GLY	3.6
1	E	613	ASP	3.5
2	H	156	GLY	3.5
1	C	400	GLU	3.5
1	C	843	GLN	3.5
1	C	686	ASP	3.5
2	B	53	ARG	3.5
1	C	668	ASP	3.4
2	B	52	ASN	3.4
2	F	45	ALA	3.4
2	H	54	LEU	3.4
1	G	844	SER	3.4
1	A	686	ASP	3.3
2	H	163	VAL	3.3
2	B	44	ALA	3.3
1	A	512	ASP	3.3
1	A	672	GLU	3.2
1	E	611	MET	3.1
1	C	624	ASP	3.1
2	F	115	ASP	3.1
2	B	46	GLY	3.1
1	A	769	ASP	3.1
1	A	610	GLU	3.1
1	C	376	GLU	3.1
1	E	273	GLU	3.1
1	C	401	GLY	3.1
1	E	844	SER	3.1
1	G	641	HIS	3.0
1	A	400	GLU	3.0
1	E	641	HIS	2.9
1	A	368	GLU	2.9
1	G	368	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	401	GLY	2.9
2	H	159	PHE	2.9
1	E	334	LYS	2.9
2	F	92	PRO	2.9
1	C	844	SER	2.9
1	A	668	ASP	2.9
2	F	156	GLY	2.9
1	E	368	GLU	2.9
1	C	121[A]	GLN	2.9
1	G	41	ASN	2.9
1	A	401	GLY	2.9
1	C	46	THR	2.9
2	F	101	THR	2.9
1	C	274	ALA	2.9
1	G	672	GLU	2.8
2	F	73	GLU	2.8
1	A	624	ASP	2.8
1	C	340	GLY	2.8
2	H	101	THR	2.8
1	C	273	GLU	2.8
2	H	53	ARG	2.8
2	D	116	ASN	2.8
2	H	153	ALA	2.8
1	G	265	GLU	2.8
1	G	256	ARG	2.8
1	G	46	THR	2.8
2	B	47	VAL	2.8
2	D	58	SER	2.7
1	A	641	HIS	2.7
2	H	124	HIS	2.7
1	E	672	GLU	2.7
1	G	340	GLY	2.7
1	A	265	GLU	2.7
2	H	61	THR	2.7
2	B	50	PRO	2.7
1	E	329	ARG	2.7
1	A	62	GLN	2.7
1	G	669	GLY	2.7
1	G	751	GLU	2.7
1	C	644	GLU	2.6
1	C	334	LYS	2.6
2	H	52	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	341	THR	2.6
1	E	512	ASP	2.6
1	E	769	ASP	2.6
2	F	57	ILE	2.6
1	C	256	ARG	2.6
1	G	339	GLU	2.6
2	H	56	ASN	2.6
1	E	256	ARG	2.6
2	H	165	GLU	2.6
2	D	115	ASP	2.6
2	B	48	GLU	2.6
1	G	523	GLU	2.5
1	G	402	GLY	2.5
2	H	58	SER	2.5
2	F	102	ILE	2.5
1	E	830	ARG	2.5
2	D	175	LEU	2.5
2	B	153	ALA	2.5
1	A	41	ASN	2.5
1	G	670	LYS	2.5
2	B	155	ASN	2.5
1	E	49	GLN	2.4
2	F	155	ASN	2.4
1	C	379	GLU	2.4
1	G	64	GLU	2.4
1	E	402	GLY	2.4
2	D	94	GLY	2.4
1	G	830	ARG	2.4
1	A	751	GLU	2.4
1	G	624	ASP	2.4
1	A	341	THR	2.4
1	C	512	ASP	2.4
2	B	154	ASP	2.4
1	C	268	PRO	2.4
1	A	273	GLU	2.3
1	C	531	ASP	2.3
1	G	512	ASP	2.3
2	H	95	ASP	2.3
2	D	92	PRO	2.3
1	A	264	LYS	2.3
1	A	478	GLN	2.3
1	C	62	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	293	GLN	2.3
1	C	626	GLN	2.3
1	A	58	SER	2.3
1	C	830	ARG	2.3
2	H	164	ASP	2.3
2	H	55	ALA	2.2
1	C	523	GLU	2.2
2	H	73	GLU	2.2
1	A	330	ASP	2.2
2	H	168	TYR	2.2
2	F	116	ASN	2.2
1	G	478	GLN	2.2
1	C	769	ASP	2.2
1	G	403	LYS	2.2
1	A	48	PRO	2.2
1	G	613	ASP	2.2
1	E	751	GLU	2.2
1	A	449	GLY	2.2
1	G	668	ASP	2.2
2	F	124	HIS	2.2
1	G	733	GLU	2.1
1	E	707	GLN	2.1
2	B	175	LEU	2.1
1	A	402	GLY	2.1
1	E	668	ASP	2.1
1	G	769	ASP	2.1
1	C	339	GLU	2.1
1	E	644	GLU	2.1
1	C	522	ARG	2.1
1	E	403	LYS	2.1
2	H	123	GLY	2.1
2	F	58	SER	2.1
1	C	368	GLU	2.1
1	G	261	GLY	2.1
1	E	270	GLU	2.0
1	G	334	LYS	2.0
1	G	268	PRO	2.0
1	G	62	GLN	2.0
1	E	115	GLU	2.0
2	B	159	PHE	2.0
1	E	274	ALA	2.0
1	A	92	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	57	ILE	2.0
2	B	152	VAL	2.0
2	D	85	ARG	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, 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
4	O	G	2003	1/1	0.90	0.18	56,56,56,56	0
4	O	E	2003	1/1	0.92	0.14	57,57,57,57	0
4	O	A	2003	1/1	0.92	0.15	55,55,55,55	0
7	FES	H	2006	4/4	0.95	0.14	81,81,82,88	0
4	O	C	2003	1/1	0.97	0.11	56,56,56,56	0
3	MGD	E	2001	47/47	0.97	0.08	53,54,57,57	0
3	MGD	G	2001	47/47	0.97	0.08	52,55,57,58	0
7	FES	F	2006	4/4	0.97	0.11	74,76,77,84	0
3	MGD	A	2001	47/47	0.97	0.09	51,53,54,55	0
3	MGD	A	2002	47/47	0.98	0.08	48,51,51,52	0
3	MGD	E	2002	47/47	0.98	0.08	52,53,56,57	0
3	MGD	C	2001	47/47	0.98	0.08	52,53,54,55	0
7	FES	B	2006	4/4	0.98	0.12	74,79,82,85	0
7	FES	D	2006	4/4	0.98	0.09	79,80,83,86	0
3	MGD	G	2002	47/47	0.98	0.07	53,55,58,59	0
3	MGD	C	2002	47/47	0.98	0.07	50,52,55,55	0
6	F3S	A	2005	7/7	0.99	0.04	53,54,55,55	0
6	F3S	C	2005	7/7	0.99	0.04	54,55,56,57	0
6	F3S	E	2005	7/7	0.99	0.03	56,56,57,57	0
6	F3S	G	2005	7/7	0.99	0.04	56,57,57,57	0

Continued on next page...

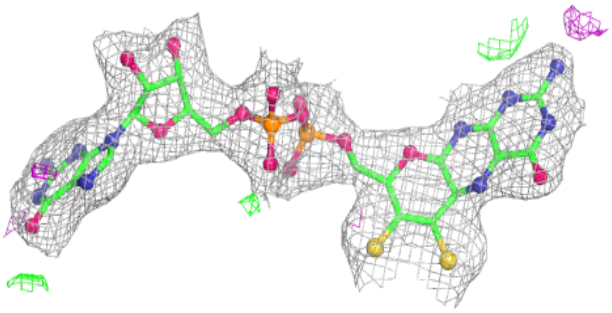
Continued from previous page...

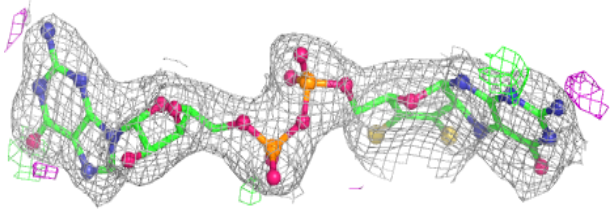
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	4MO	A	2004	1/1	1.00	0.02	53,53,53,53	0
5	4MO	C	2004	1/1	1.00	0.03	54,54,54,54	0
5	4MO	E	2004	1/1	1.00	0.03	57,57,57,57	0
5	4MO	G	2004	1/1	1.00	0.02	56,56,56,56	0

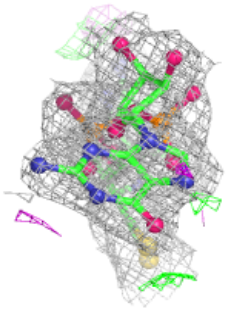
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD E 2001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

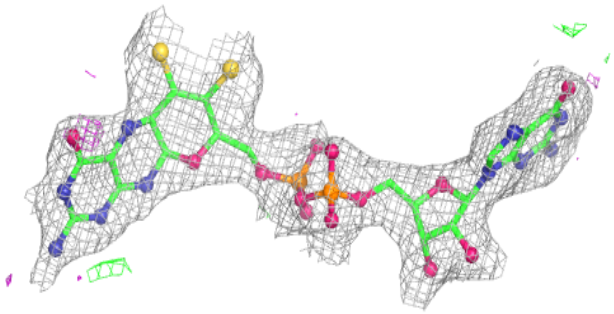


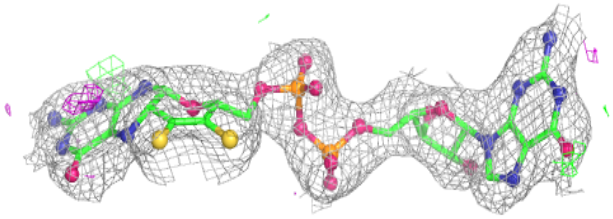


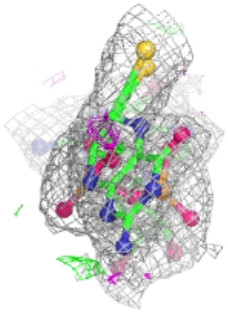


Electron density around MGD G 2001:

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

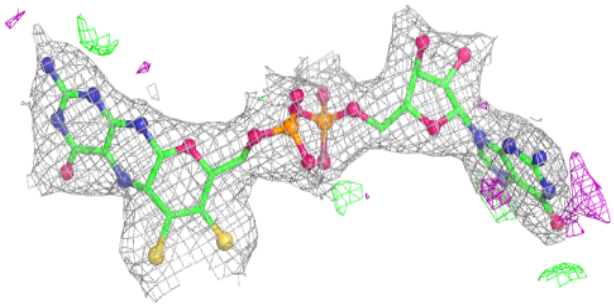


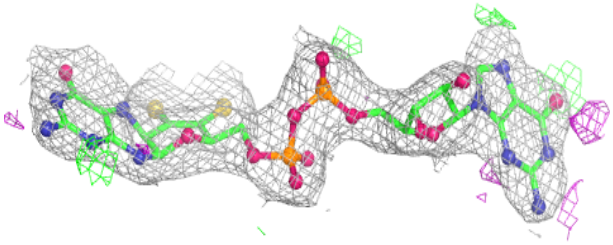


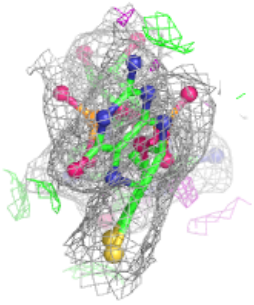


Electron density around MGD A 2001:

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

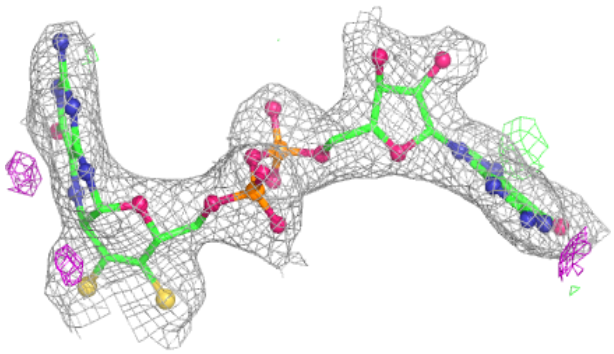


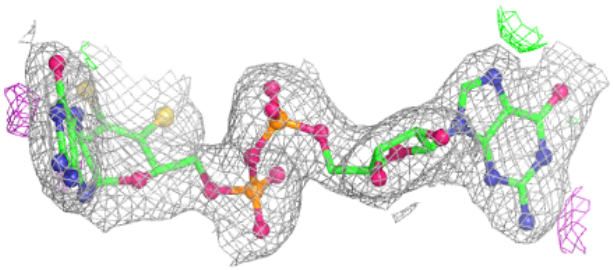


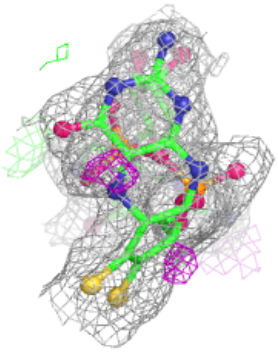


Electron density around MGD A 2002:

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

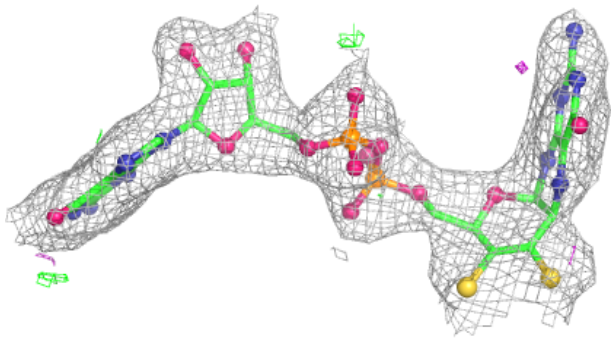


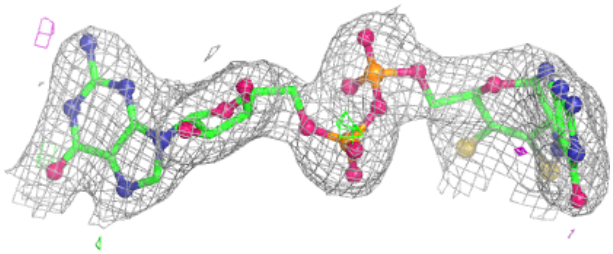


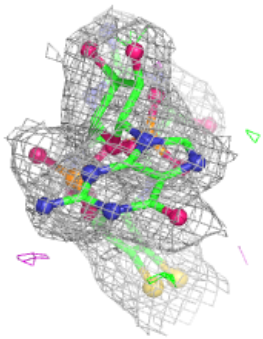


Electron density around MGD E 2002:

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

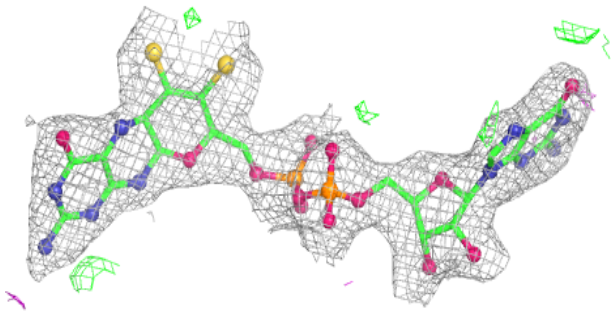


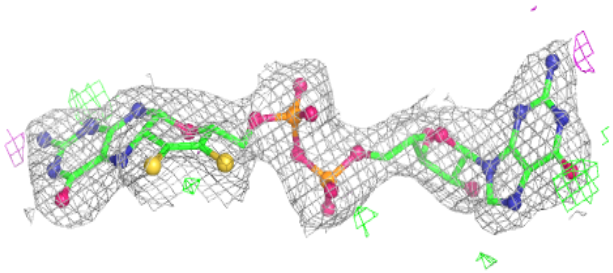


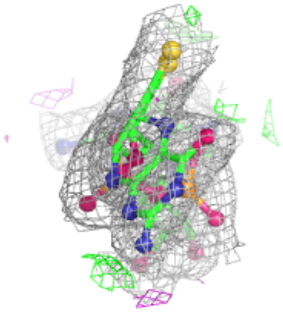


Electron density around MGD C 2001:

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

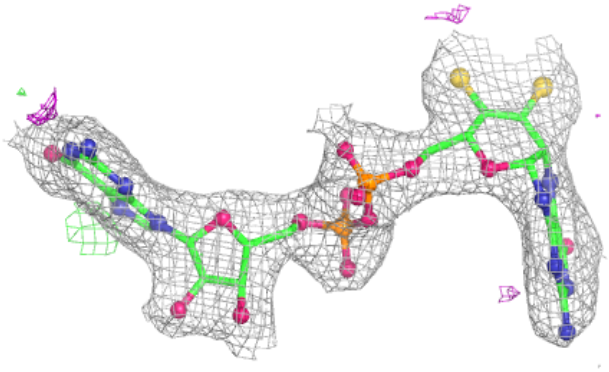


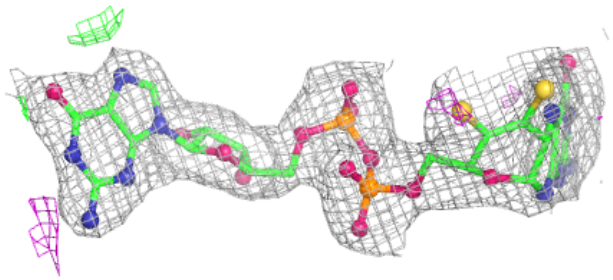


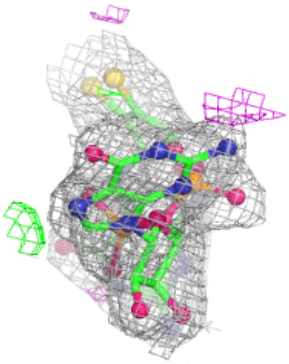


Electron density around MGD G 2002:

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

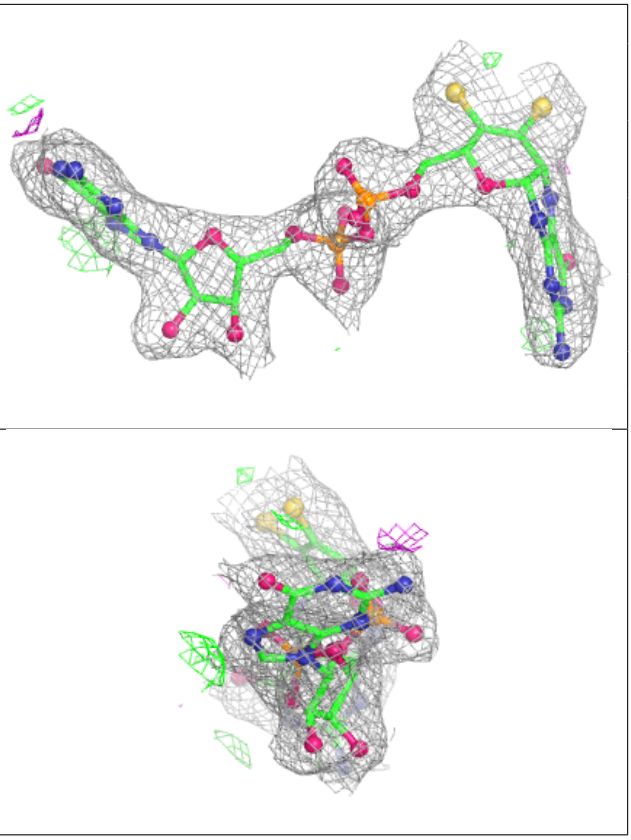






Electron density around MGD C 2002:

$2mF_o$-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.