Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 07:22 AM EDT

PDB ID	:	4DP3
Title	:	Quadruple mutant (N51I+C59R+S108N+I164L) plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with P218 and NADPH
Authors	:	Yuthavong, Y.; Vilaivan, T.; Kamchonwongpaisan, S.; Charman, S.A.; McLennan, D.N.; White, K.L.; Vivas, L.; Bongard, E.; Chitnumsub, P.; Tarnchompoo, B.; Thongphanchang, C.; Taweechai, S.; Vanichtanakul, J.; Arwon, U.; Fantauzzi, P.; Yuvaniyama, J.; Charman, W.N.; Matthews, D.
Deposited on	:	2012-02-13
Resolution	:	2.40 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:

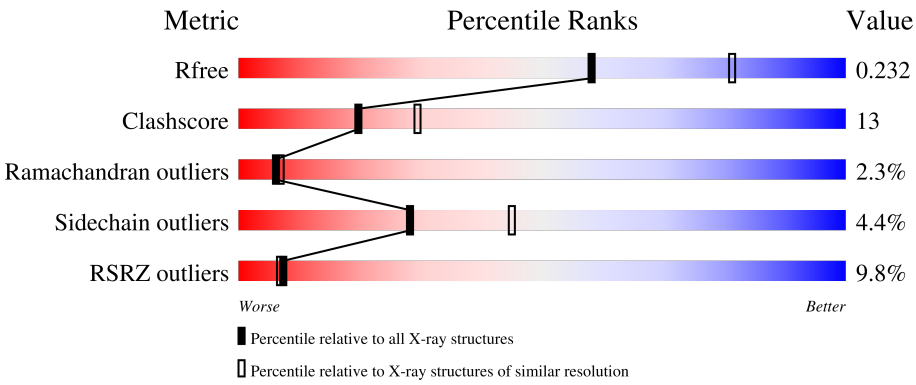
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)

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 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	608	7% 68% 19% • 10%
1	B	608	11% 63% 23% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	A	703	-	X	-	-
4	PO4	B	703	-	X	-	-

2 Entry composition (i)

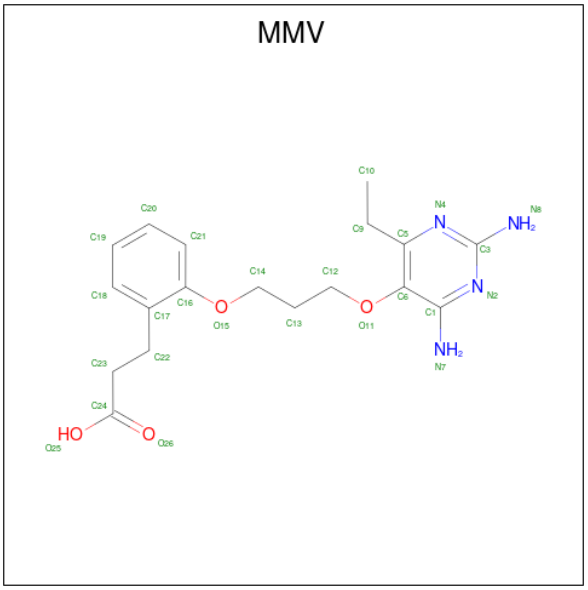
There are 5 unique types of molecules in this entry. The entry contains 9667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional dihydrofolate reductase-thymidylate synthase.

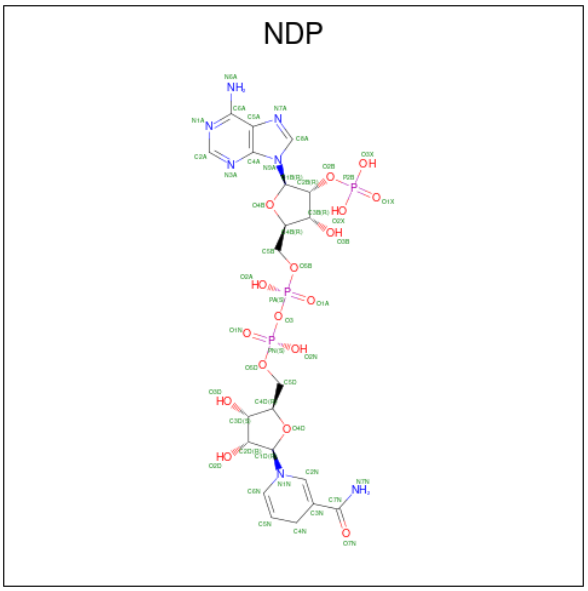
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	4539	2931	751	830	27	0	0	0
1	B	544	4529	2924	751	828	26	0	0	0

- Molecule 2 is 3-(2-{3-[(2,4-diamino-6-ethylpyrimidin-5-yl)oxy]propoxy}phenyl)propanoic acid (three-letter code: MMV) (formula: $C_{18}H_{24}N_4O_4$).



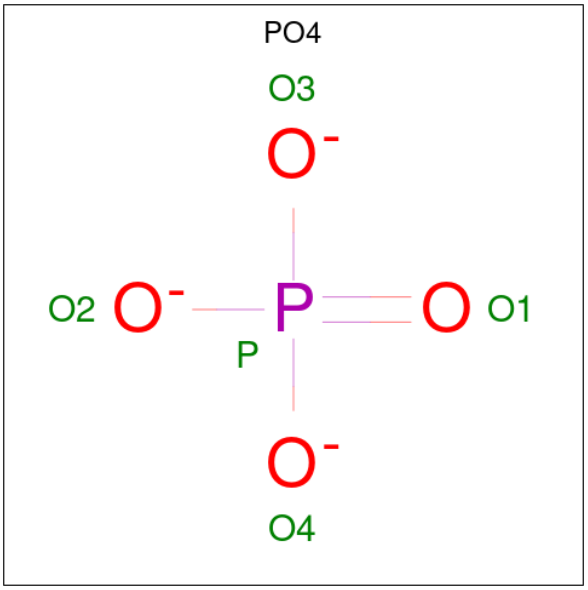
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	26	18	4	4	0	0
2	B	1	26	18	4	4	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 5 is water.

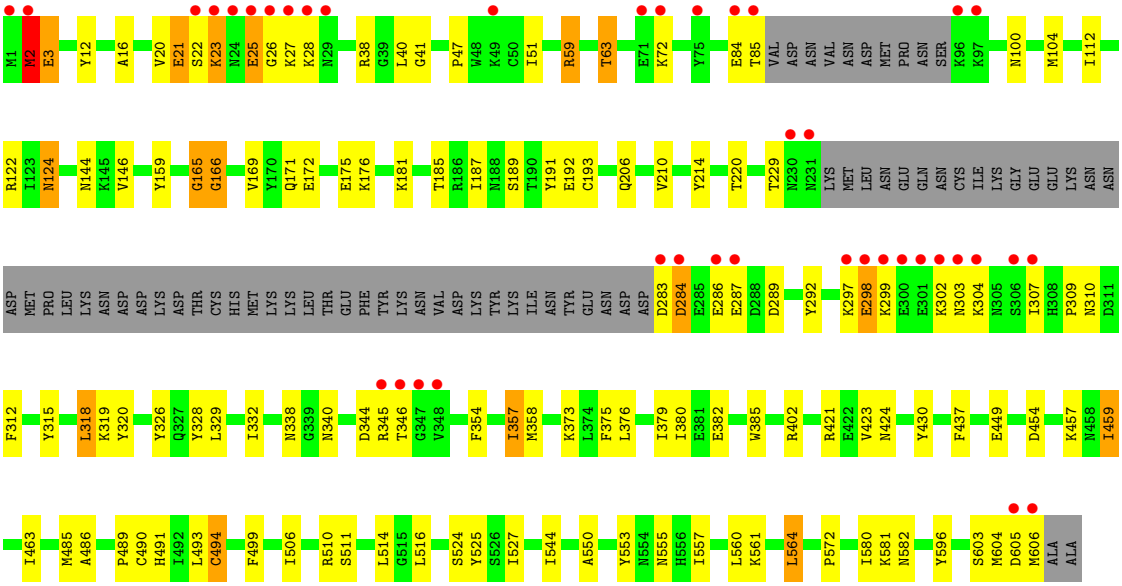
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	233	233	233	0	0
			Total	O		
5	B	208	208	208	0	0

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.

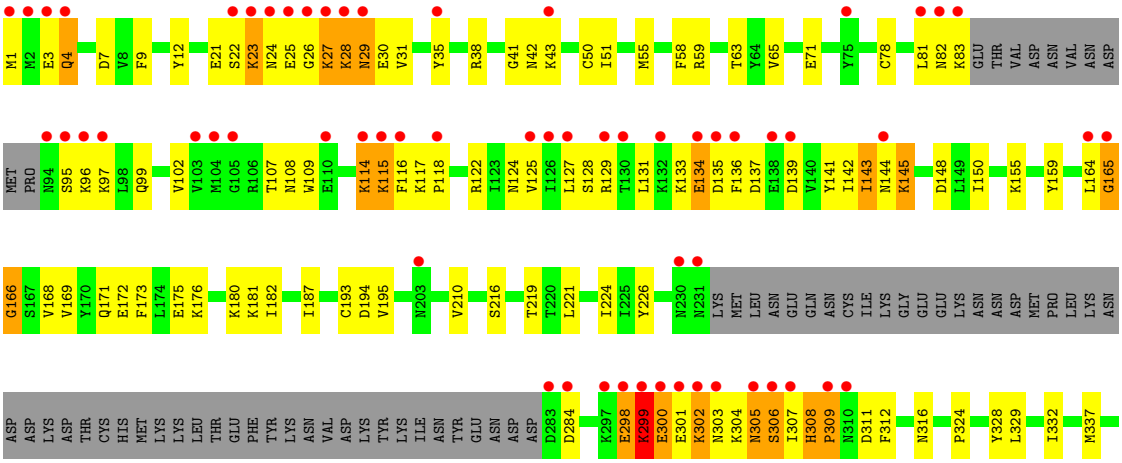
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

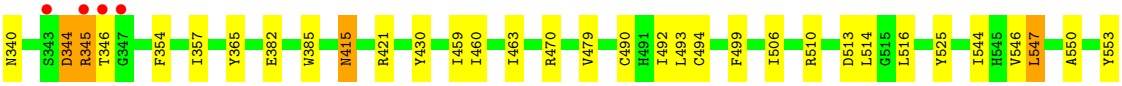
Chain A:

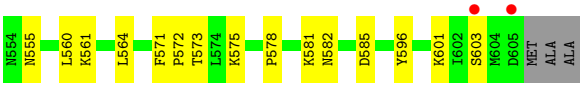


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain B:




N340
S343
D344
R345
T346
G347
F354
I357
Y365
E382
W385
N415
R421
Y430
I459
I460
I463
R470
V479
C490
H491
I492
L493
C494
F499
I506
R510
D513
L514
G515
L516
Y525
I544
H545
V546
L547
A550
Y553


N554
N555
L560
K561
L564
F571
P572
T573
L574
K575
P578
K581
N582
D585
Y596
K601
I602
S603
M604
D605
MET
ALA
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.50Å 156.20Å 164.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.40 19.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.5 (19.90-2.40) 96.6 (19.90-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.28 (at 2.41Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.205 , 0.239 0.199 , 0.232	Depositor DCC
R_{free} test set	2903 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9667	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: NDP, MMV, PO4

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	0.39	1/4644 (0.0%)	0.71	2/6267 (0.0%)
1	B	0.38	0/4634	0.72	6/6254 (0.1%)
All	All	0.39	1/9278 (0.0%)	0.72	8/12521 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	494	CYS	CB-SG	-5.06	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	GLY	N-CA-C	-10.23	87.53	113.10
1	B	165	GLY	N-CA-C	7.31	131.38	113.10
1	B	300	GLU	N-CA-C	-6.50	93.45	111.00
1	B	166	GLY	N-CA-C	-6.45	96.99	113.10
1	A	165	GLY	N-CA-C	5.93	127.92	113.10
1	B	299	LYS	N-CA-C	5.32	125.36	111.00
1	B	26	GLY	N-CA-C	-5.21	100.07	113.10
1	B	305	ASN	N-CA-C	-5.01	97.48	111.00

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	4539	0	4501	94	0
1	B	4529	0	4490	144	0
2	A	26	0	23	1	0
2	B	26	0	23	0	0
3	A	48	0	26	3	0
3	B	48	0	26	5	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	A	233	0	0	6	0
5	B	208	0	0	12	0
All	All	9667	0	9089	232	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 13.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLU:C	1:B:303:ASN:H	1.48	1.06
1:B:490:CYS:SG	5:B:989:HOH:O	2.21	0.96
1:B:299:LYS:C	1:B:301:GLU:H	1.64	0.91
1:A:51:ILE:HD13	1:A:187:ILE:HD12	1.53	0.89
1:B:137:ASP:HB3	5:B:895:HOH:O	1.78	0.83
1:A:59:ARG:O	1:A:63:THR:HG23	1.79	0.82
1:B:299:LYS:HG3	1:B:301:GLU:HA	1.61	0.81
1:B:301:GLU:C	1:B:303:ASN:N	2.26	0.80
1:A:329:LEU:HD22	1:A:564:LEU:HD12	1.64	0.78
1:A:298:GLU:HG3	1:A:299:LYS:O	1.84	0.77
1:B:299:LYS:HE2	1:B:301:GLU:HB3	1.66	0.76
1:A:302:LYS:O	1:A:302:LYS:HG2	1.86	0.74
1:B:415:ASN:HB2	5:B:894:HOH:O	1.86	0.74
1:A:166:GLY:HA3	3:A:702:NDP:PA	2.28	0.74
1:B:59:ARG:O	1:B:63:THR:HG23	1.91	0.71
1:B:573:THR:HG23	5:B:879:HOH:O	1.88	0.71
1:A:454:ASP:OD2	1:A:457:LYS:HG3	1.91	0.70
1:B:4:GLN:HB3	1:B:7:ASP:OD2	1.92	0.69
1:B:494:CYS:SG	1:B:525:TYR:HE2	2.15	0.69
1:A:376:LEU:HD22	1:A:379:ILE:HD11	1.75	0.69
1:B:582:ASN:HB3	5:B:901:HOH:O	1.93	0.68
1:B:299:LYS:C	1:B:301:GLU:N	2.37	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HB2	1:B:148:ASP:OD2	1.93	0.67
1:B:65:VAL:HG22	1:B:159:TYR:CB	2.24	0.67
1:B:108:ASN:ND2	1:B:165:GLY:O	2.28	0.67
1:A:490:CYS:SG	5:A:1016:HOH:O	2.53	0.66
1:B:81:LEU:CD2	1:B:83:LYS:HE2	2.26	0.66
1:B:42:ASN:HB2	1:B:193:CYS:HA	1.78	0.66
1:B:345:ARG:HD3	5:B:876:HOH:O	1.97	0.65
1:B:506:ILE:HG12	1:B:544:ILE:HB	1.79	0.65
1:A:21:GLU:HB2	5:A:994:HOH:O	1.96	0.65
1:B:131:LEU:HD22	1:B:136:PHE:HE2	1.60	0.65
1:B:304:LYS:HD3	1:B:337:MET:O	1.96	0.65
1:B:415:ASN:C	1:B:415:ASN:HD22	2.00	0.64
1:B:166:GLY:HA3	3:B:702:NDP:PA	2.38	0.64
1:A:171:GLN:O	1:A:175:GLU:HG3	1.97	0.64
1:B:332:ILE:HD13	1:B:560:LEU:HD22	1.79	0.64
1:B:51:ILE:HD13	1:B:187:ILE:HD12	1.81	0.63
1:A:2:MET:O	1:A:2:MET:SD	2.56	0.63
1:A:100:ASN:OD1	1:A:159:TYR:HB3	1.98	0.63
1:A:328:TYR:CZ	1:A:332:ILE:HD11	2.32	0.63
1:B:306:SER:C	1:B:307:ILE:HG12	2.19	0.62
1:A:494:CYS:SG	1:A:525:TYR:HE2	2.22	0.62
1:B:182:ILE:HB	1:B:226:TYR:HB2	1.81	0.61
1:B:299:LYS:HE3	1:B:301:GLU:HB2	1.82	0.61
1:B:299:LYS:CE	1:B:301:GLU:HB3	2.30	0.61
1:B:299:LYS:O	1:B:299:LYS:HG2	2.00	0.61
1:B:114:LYS:HB2	5:B:931:HOH:O	2.01	0.59
1:A:124:ASN:N	1:A:124:ASN:HD22	1.99	0.59
1:B:23:LYS:O	1:B:25:GLU:N	2.32	0.59
1:A:72:LYS:NZ	1:A:72:LYS:HB3	2.17	0.59
1:B:81:LEU:HG	1:B:83:LYS:HE2	1.85	0.59
1:A:582:ASN:HB2	5:A:949:HOH:O	2.01	0.58
1:B:23:LYS:C	1:B:25:GLU:H	2.07	0.58
1:B:575:LYS:HG3	5:B:1003:HOH:O	2.03	0.58
1:A:454:ASP:CG	1:A:457:LYS:HG3	2.25	0.57
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.39	0.57
1:B:301:GLU:O	1:B:303:ASN:N	2.34	0.57
1:A:354:PHE:CE2	1:B:506:ILE:HG13	2.39	0.57
1:B:299:LYS:CE	1:B:301:GLU:CB	2.82	0.57
1:B:136:PHE:CD2	1:B:142:ILE:HD11	2.39	0.56
1:B:169:VAL:O	1:B:173:PHE:HD2	1.88	0.56
1:B:494:CYS:SG	1:B:525:TYR:CE2	2.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LYS:HE3	1:B:116:PHE:CZ	2.41	0.56
1:A:51:ILE:CD1	1:A:187:ILE:HD12	2.32	0.56
1:B:470:ARG:HD3	5:B:888:HOH:O	2.05	0.55
1:A:506:ILE:HG13	1:B:354:PHE:CE2	2.41	0.55
1:B:1:MET:HE2	1:B:1:MET:HA	1.88	0.55
1:B:357:ILE:CD1	1:B:546:VAL:HG22	2.37	0.55
1:A:494:CYS:SG	1:A:525:TYR:CE2	3.00	0.55
1:B:210:VAL:HG12	1:B:224:ILE:HG22	1.89	0.55
1:A:493:LEU:C	1:A:493:LEU:HD12	2.26	0.55
1:B:171:GLN:O	1:B:175:GLU:HG2	2.06	0.55
1:A:307:ILE:HG21	1:A:312:PHE:HE2	1.72	0.54
1:B:300:GLU:OE1	1:B:302:LYS:HE3	2.07	0.54
1:A:373:LYS:HE2	1:A:375:PHE:CZ	2.42	0.54
1:A:22:SER:C	1:A:23:LYS:HG2	2.28	0.54
1:A:284:ASP:HB2	1:A:287:GLU:OE1	2.08	0.54
1:A:312:PHE:CE1	1:A:564:LEU:HD23	2.43	0.54
1:B:493:LEU:HD12	1:B:493:LEU:C	2.29	0.54
1:A:16:ALA:HA	1:A:185:THR:HB	1.90	0.53
1:B:299:LYS:HG3	1:B:301:GLU:CA	2.34	0.53
1:B:575:LYS:CG	5:B:1003:HOH:O	2.56	0.53
1:B:298:GLU:HG2	1:B:299:LYS:N	2.23	0.53
1:A:146:VAL:HG21	1:A:176:LYS:HE3	1.90	0.52
1:A:357:ILE:HD13	1:A:357:ILE:C	2.30	0.52
1:B:547:LEU:N	1:B:547:LEU:HD23	2.25	0.52
1:B:58:PHE:CE1	1:B:164:LEU:HD22	2.45	0.52
1:B:308:HIS:ND1	1:B:308:HIS:N	2.56	0.52
1:B:95:SER:OG	1:B:96:LYS:N	2.43	0.52
1:A:340:ASN:HB3	1:B:499:PHE:CE1	2.45	0.52
1:A:63:THR:HG22	1:A:122:ARG:HD3	1.91	0.51
1:B:108:ASN:HB2	1:B:165:GLY:O	2.10	0.51
1:A:376:LEU:HD13	1:A:527:ILE:HD11	1.92	0.51
1:B:555:ASN:HB3	5:B:963:HOH:O	2.11	0.51
1:A:112:ILE:HD11	2:A:701:MMV:H15	1.91	0.51
1:B:299:LYS:HE2	1:B:301:GLU:CB	2.37	0.51
1:A:63:THR:HG22	1:A:122:ARG:CD	2.39	0.51
1:A:192:GLU:HA	5:A:994:HOH:O	2.10	0.51
1:B:95:SER:O	1:B:96:LYS:HG2	2.10	0.50
1:B:134:GLU:C	1:B:136:PHE:H	2.14	0.50
1:B:144:ASN:O	3:B:702:NDP:H2A	2.12	0.50
1:B:169:VAL:HG23	3:B:702:NDP:O1A	2.10	0.50
1:A:485:MET:SD	1:A:489:PRO:HD3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:PHE:HB2	1:B:316:ASN:ND2	2.26	0.50
1:B:305:ASN:N	5:B:1008:HOH:O	2.45	0.49
1:B:129:ARG:HB2	3:B:702:NDP:O3X	2.13	0.49
1:A:206:GLN:HG2	1:A:229:THR:HG22	1.94	0.48
1:B:81:LEU:CG	1:B:83:LYS:HE2	2.42	0.48
1:A:572:PRO:HB3	1:A:596:TYR:HA	1.95	0.48
1:B:168:VAL:O	1:B:172:GLU:HG2	2.13	0.48
1:A:423:VAL:O	1:A:424:ASN:HB2	2.14	0.48
1:B:29:ASN:O	1:B:30:GLU:C	2.52	0.48
1:B:28:LYS:HG3	1:B:29:ASN:N	2.29	0.48
1:B:43:LYS:H	1:B:194:ASP:CG	2.17	0.48
1:B:303:ASN:C	1:B:304:LYS:HG3	2.33	0.48
1:B:21:GLU:C	1:B:23:LYS:H	2.17	0.48
1:B:58:PHE:HE1	1:B:164:LEU:HD22	1.78	0.48
1:A:214:TYR:O	1:A:220:THR:HA	2.14	0.47
1:B:141:TYR:N	1:B:141:TYR:CD2	2.82	0.47
1:B:115:LYS:HE3	1:B:116:PHE:CE2	2.49	0.47
1:A:307:ILE:CG2	1:A:312:PHE:HE2	2.26	0.47
1:B:102:VAL:HG11	1:B:122:ARG:HD2	1.96	0.47
1:A:315:TYR:HB2	1:A:564:LEU:O	2.14	0.47
1:B:572:PRO:HB3	1:B:596:TYR:HA	1.96	0.47
1:B:345:ARG:NH2	4:B:703:PO4:O1	2.47	0.47
1:A:332:ILE:HD13	1:A:560:LEU:HD22	1.96	0.47
1:B:145:LYS:HA	3:B:702:NDP:N1A	2.29	0.47
1:B:78:CYS:O	1:B:82:ASN:N	2.47	0.46
1:B:308:HIS:O	1:B:311:ASP:HB2	2.15	0.46
1:B:1:MET:HA	1:B:1:MET:CE	2.45	0.46
1:B:300:GLU:CD	1:B:302:LYS:HE3	2.36	0.46
1:B:328:TYR:CZ	1:B:332:ILE:HD11	2.51	0.46
1:A:289:ASP:HA	1:A:292:TYR:CD2	2.50	0.46
1:A:373:LYS:HE2	1:A:375:PHE:CE2	2.51	0.46
1:A:297:LYS:O	1:A:298:GLU:O	2.34	0.46
1:A:382:GLU:O	1:A:385:TRP:HB3	2.14	0.46
1:B:301:GLU:O	1:B:301:GLU:HG3	2.16	0.46
1:A:165:GLY:HA2	1:A:169:VAL:HB	1.97	0.46
1:B:102:VAL:HB	1:B:164:LEU:HD11	1.97	0.46
1:B:299:LYS:HE3	1:B:301:GLU:CB	2.43	0.46
1:B:553:TYR:HB3	1:B:555:ASN:OD1	2.15	0.46
1:B:65:VAL:HG22	1:B:159:TYR:HB2	1.97	0.46
1:B:382:GLU:O	1:B:385:TRP:HB3	2.16	0.46
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:CYS:N	5:A:994:HOH:O	2.48	0.45
1:B:459:ILE:HG13	1:B:460:ILE:N	2.31	0.45
1:A:580:ILE:O	1:A:581:LYS:HD3	2.16	0.45
1:B:109:TRP:CZ2	1:B:117:LYS:HD2	2.51	0.45
1:B:136:PHE:CE2	1:B:142:ILE:HD11	2.52	0.45
1:B:141:TYR:H	1:B:141:TYR:HD2	1.63	0.45
1:A:357:ILE:HD13	1:A:358:MET:N	2.31	0.45
1:B:63:THR:HG22	1:B:122:ARG:CD	2.46	0.45
1:B:578:PRO:O	1:B:581:LYS:HE3	2.16	0.45
1:A:319:LYS:HG3	1:A:320:TYR:CD2	2.51	0.45
1:A:2:MET:O	1:A:3:GLU:C	2.54	0.44
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.99	0.44
1:A:485:MET:O	1:A:486:ALA:C	2.54	0.44
1:B:329:LEU:HD22	1:B:564:LEU:HD12	1.99	0.44
1:A:166:GLY:HA3	3:A:702:NDP:O1A	2.17	0.44
1:A:506:ILE:HG12	1:A:544:ILE:HB	2.00	0.44
1:A:210:VAL:HG21	1:A:326:TYR:HE2	1.82	0.44
1:B:35:TYR:CZ	1:B:38:ARG:HD3	2.53	0.44
1:B:65:VAL:HG22	1:B:159:TYR:HB3	1.97	0.44
1:B:12:TYR:CE1	1:B:180:LYS:HB3	2.53	0.44
1:B:43:LYS:N	1:B:194:ASP:OD2	2.44	0.44
1:B:216:SER:O	1:B:219:THR:HG22	2.18	0.44
1:B:118:PRO:HB2	1:B:124:ASN:ND2	2.32	0.44
1:B:312:PHE:CE1	1:B:561:LYS:HG2	2.53	0.44
1:A:421:ARG:HG2	1:A:421:ARG:HH11	1.83	0.44
1:B:1:MET:C	1:B:3:GLU:H	2.19	0.44
1:B:299:LYS:CG	1:B:301:GLU:CA	2.96	0.44
1:A:172:GLU:O	1:A:176:LYS:HG3	2.17	0.43
1:A:499:PHE:CE1	1:B:340:ASN:HB3	2.54	0.43
1:B:172:GLU:O	1:B:176:LYS:HG3	2.17	0.43
1:B:307:ILE:CG2	1:B:312:PHE:CE2	3.01	0.43
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.83	0.43
1:A:516:LEU:HD21	1:A:604:MET:CG	2.48	0.43
1:A:553:TYR:HB3	1:A:555:ASN:OD1	2.18	0.43
1:B:459:ILE:O	1:B:463:ILE:HG13	2.19	0.43
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.54	0.43
1:A:437:PHE:CD1	1:B:479:VAL:HB	2.53	0.43
1:B:131:LEU:HD22	1:B:136:PHE:CE2	2.48	0.43
1:A:318:LEU:N	1:A:318:LEU:HD23	2.34	0.43
1:B:9:PHE:CE2	1:B:150:ILE:HG23	2.54	0.43
1:A:22:SER:O	1:A:25:GLU:OE1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:O	1:A:47:PRO:HD3	2.18	0.42
1:A:603:SER:HA	5:A:1015:HOH:O	2.19	0.42
1:B:513:ASP:OD2	1:B:516:LEU:HB2	2.19	0.42
1:B:97:LYS:O	1:B:99:GLN:HG3	2.19	0.42
1:B:514:LEU:HD21	1:B:550:ALA:HB1	2.00	0.42
1:A:72:LYS:HB3	1:A:72:LYS:HZ3	1.81	0.42
1:A:166:GLY:HA3	3:A:702:NDP:O2A	2.18	0.42
1:A:376:LEU:O	1:A:380:ILE:HG13	2.17	0.42
1:A:510:ARG:HG3	1:A:511:SER:N	2.34	0.42
1:A:557:ILE:O	1:A:561:LYS:HG3	2.19	0.42
1:A:560:LEU:HG	1:A:604:MET:CE	2.50	0.42
1:B:134:GLU:H	1:B:134:GLU:HG2	1.57	0.42
1:B:41:GLY:O	1:B:193:CYS:HB3	2.20	0.42
1:A:22:SER:HB2	1:A:25:GLU:CD	2.40	0.42
1:B:344:ASP:O	1:B:346:THR:N	2.52	0.42
1:B:128:SER:HB3	1:B:131:LEU:HB2	2.02	0.42
1:B:299:LYS:CE	1:B:301:GLU:HB2	2.46	0.42
1:B:307:ILE:HG23	1:B:561:LYS:HE2	2.00	0.42
1:A:514:LEU:HD21	1:A:550:ALA:HB1	2.02	0.42
1:B:221:LEU:HD23	1:B:221:LEU:N	2.35	0.42
1:B:303:ASN:O	1:B:304:LYS:HG3	2.20	0.42
1:B:492:ILE:HD11	1:B:510:ARG:HD3	2.02	0.42
1:B:582:ASN:HB2	1:B:585:ASP:OD2	2.20	0.42
1:B:324:PRO:HB2	1:B:571:PHE:HE2	1.85	0.41
1:B:125:VAL:CG1	1:B:143:ILE:HD11	2.49	0.41
1:A:20:VAL:HG11	1:A:38:ARG:HG3	2.02	0.41
1:B:155:LYS:HE3	1:B:155:LYS:HB2	1.88	0.41
1:A:459:ILE:O	1:A:463:ILE:HG13	2.20	0.41
1:B:415:ASN:O	1:B:415:ASN:ND2	2.42	0.41
1:A:303:ASN:ND2	1:A:338:ASN:OD1	2.54	0.41
1:A:63:THR:HG22	1:A:122:ARG:NE	2.36	0.41
1:A:516:LEU:CD2	1:A:604:MET:HG3	2.50	0.41
1:B:357:ILE:HD13	1:B:546:VAL:HG22	2.03	0.41
1:A:344:ASP:O	1:A:346:THR:N	2.54	0.41
1:A:560:LEU:HG	1:A:604:MET:HE1	2.02	0.41
1:B:306:SER:O	1:B:307:ILE:HG12	2.21	0.41
1:B:324:PRO:HG2	1:B:365:TYR:CZ	2.56	0.41
1:A:499:PHE:CZ	1:B:340:ASN:HB3	2.56	0.41
1:A:604:MET:HB3	1:A:604:MET:HE3	1.97	0.41
1:B:63:THR:HG22	1:B:122:ARG:NE	2.37	0.40
1:B:309:PRO:C	1:B:311:ASP:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:SER:HG	1:A:191:TYR:HE2	1.69	0.40
1:A:210:VAL:O	1:A:210:VAL:HG23	2.20	0.40
1:B:284:ASP:OD1	1:B:284:ASP:N	2.53	0.40
1:A:283:ASP:OD1	1:A:284:ASP:N	2.54	0.40
1:A:493:LEU:HD12	1:A:493:LEU:O	2.21	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	539/608 (89%)	507 (94%)	21 (4%)	11 (2%)	7 9
1	B	538/608 (88%)	484 (90%)	40 (7%)	14 (3%)	5 5
All	All	1077/1216 (89%)	991 (92%)	61 (6%)	25 (2%)	6 7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	23	LYS
1	A	298	GLU
1	A	304	LYS
1	B	28	LYS
1	B	299	LYS
1	A	3	GLU
1	A	310	ASN
1	A	345	ARG
1	A	430	TYR
1	B	22	SER
1	B	27	LYS
1	B	29	ASN

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Mol	Chain	Res	Type
1	B	115	LYS
1	B	345	ARG
1	B	430	TYR
1	A	309	PRO
1	B	114	LYS
1	B	133	LYS
1	B	302	LYS
1	A	26	GLY
1	A	284	ASP
1	B	24	ASN
1	B	298	GLU
1	B	309	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	510/570 (90%)	487 (96%)	23 (4%)	27	44
1	B	509/570 (89%)	487 (96%)	22 (4%)	29	46
All	All	1019/1140 (89%)	974 (96%)	45 (4%)	28	45

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	21	GLU
1	A	25	GLU
1	A	27	LYS
1	A	28	LYS
1	A	59	ARG
1	A	63	THR
1	A	84	GLU
1	A	85	THR
1	A	104	MET
1	A	124	ASN

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Mol	Chain	Res	Type
1	A	144	ASN
1	A	286	GLU
1	A	318	LEU
1	A	357	ILE
1	A	402	ARG
1	A	449	GLU
1	A	459	ILE
1	A	491	HIS
1	A	524	SER
1	A	564	LEU
1	A	605	ASP
1	A	606	MET
1	B	4	GLN
1	B	23	LYS
1	B	27	LYS
1	B	31	VAL
1	B	50	CYS
1	B	55	MET
1	B	71	GLU
1	B	107	THR
1	B	127	LEU
1	B	134	GLU
1	B	135	ASP
1	B	139	ASP
1	B	143	ILE
1	B	145	LYS
1	B	195	VAL
1	B	306	SER
1	B	308	HIS
1	B	344	ASP
1	B	415	ASN
1	B	547	LEU
1	B	601	LYS
1	B	603	SER

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	99	GLN
1	A	144	ASN
1	A	231	ASN
1	A	294	ASN

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Mol	Chain	Res	Type
1	A	394	ASN
1	A	407	ASN
1	A	415	ASN
1	A	424	ASN
1	A	554	ASN
1	B	94	ASN
1	B	231	ASN
1	B	316	ASN
1	B	394	ASN
1	B	415	ASN
1	B	424	ASN
1	B	551	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PO4	A	703	-	4,4,4	5.29	4 (100%)	6,6,6	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NDP	A	702	-	47,52,52	1.65	8 (17%)	61,80,80	1.86	15 (24%)
4	PO4	B	703	-	4,4,4	4.48	4 (100%)	6,6,6	0.64	0
3	NDP	B	702	-	47,52,52	1.66	7 (14%)	61,80,80	1.81	16 (26%)
2	MMV	A	701	-	27,27,27	1.12	3 (11%)	32,35,35	1.84	6 (18%)
2	MMV	B	701	-	27,27,27	1.48	6 (22%)	32,35,35	1.95	8 (25%)

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	NDP	B	702	-	-	3/30/77/77	0/5/5/5
3	NDP	A	702	-	-	4/30/77/77	0/5/5/5
2	MMV	A	701	-	-	2/15/15/15	0/2/2/2
2	MMV	B	701	-	-	4/15/15/15	0/2/2/2

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	PO4	P-O1	7.88	1.68	1.50
4	B	703	PO4	P-O2	5.02	1.69	1.54
4	A	703	PO4	P-O2	4.98	1.69	1.54
3	A	702	NDP	C4N-C3N	-4.65	1.41	1.50
4	A	703	PO4	P-O4	4.54	1.67	1.54
3	B	702	NDP	C4N-C3N	-4.45	1.41	1.50
4	B	703	PO4	P-O3	4.44	1.67	1.54
4	B	703	PO4	P-O4	4.43	1.67	1.54
3	B	702	NDP	C4N-C5N	-4.09	1.38	1.49
4	B	703	PO4	P-O1	3.96	1.59	1.50
3	A	702	NDP	C4N-C5N	-3.95	1.38	1.49
2	B	701	MMV	O26-C24	3.89	1.34	1.22
3	B	702	NDP	C2N-C3N	3.80	1.45	1.35
3	A	702	NDP	C2N-C3N	3.69	1.45	1.35
3	A	702	NDP	PA-O3	-3.36	1.55	1.59
3	A	702	NDP	P2B-O2B	-3.02	1.54	1.59
2	B	701	MMV	O25-C24	-2.86	1.21	1.30
3	B	702	NDP	P2B-O2B	-2.73	1.54	1.59
2	B	701	MMV	C16-C17	2.68	1.44	1.39
3	B	702	NDP	C3B-C2B	-2.59	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NDP	C4A-N3A	2.52	1.39	1.35
2	B	701	MMV	C3-N2	-2.37	1.31	1.35
3	A	702	NDP	C4A-N3A	2.35	1.38	1.35
2	A	701	MMV	C3-N4	-2.24	1.31	1.35
3	B	702	NDP	C6N-N1N	2.24	1.42	1.37
2	B	701	MMV	C3-N4	-2.22	1.31	1.35
3	A	702	NDP	C3B-C4B	-2.18	1.47	1.53
2	A	701	MMV	C3-N2	-2.15	1.31	1.35
3	A	702	NDP	O4B-C1B	2.11	1.43	1.40
4	A	703	PO4	P-O3	2.07	1.60	1.54
2	A	701	MMV	C16-C17	2.07	1.43	1.39
2	B	701	MMV	C1-N2	-2.01	1.32	1.35

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	MMV	C3-N4-C5	6.52	121.02	116.26
3	A	702	NDP	C4B-O4B-C1B	-5.92	104.51	109.92
2	B	701	MMV	C3-N4-C5	5.66	120.39	116.26
3	B	702	NDP	C4B-O4B-C1B	-4.76	105.57	109.92
3	A	702	NDP	O4B-C1B-N9A	4.61	114.86	108.75
3	B	702	NDP	C3N-C2N-N1N	-4.37	116.78	123.20
3	B	702	NDP	C1D-N1N-C2N	-4.36	113.95	121.14
3	A	702	NDP	C1D-N1N-C2N	-4.30	114.06	121.14
3	A	702	NDP	C3N-C2N-N1N	-4.24	116.98	123.20
2	B	701	MMV	O25-C24-C23	3.97	126.55	114.00
2	B	701	MMV	O26-C24-C23	-3.95	110.57	123.09
3	A	702	NDP	C3B-C2B-C1B	-3.89	95.35	102.81
3	B	702	NDP	O4B-C1B-N9A	3.78	113.75	108.75
3	B	702	NDP	O3B-C3B-C4B	3.33	120.65	111.08
2	B	701	MMV	C3-N2-C1	3.23	121.16	117.28
3	A	702	NDP	O7N-C7N-N7N	-3.08	115.99	122.89
3	B	702	NDP	O7N-C7N-N7N	-3.04	116.08	122.89
3	A	702	NDP	C6N-N1N-C2N	2.92	122.45	119.32
2	A	701	MMV	N4-C3-N2	-2.92	121.01	125.48
3	B	702	NDP	O3B-C3B-C2B	2.90	119.29	111.19
2	B	701	MMV	N4-C3-N2	-2.88	121.07	125.48
2	A	701	MMV	C3-N2-C1	2.87	120.72	117.28
3	B	702	NDP	C3B-C2B-C1B	-2.83	97.40	102.81
2	B	701	MMV	O15-C16-C17	2.82	119.53	115.89
3	B	702	NDP	C2B-C3B-C4B	2.81	108.03	101.99
3	A	702	NDP	C3D-C2D-C1D	-2.81	96.15	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	MMV	C23-C22-C17	2.77	120.27	112.71
2	A	701	MMV	C14-O15-C16	2.74	124.31	117.69
3	B	702	NDP	C6N-N1N-C2N	2.71	122.21	119.32
3	A	702	NDP	O3B-C3B-C2B	2.70	118.74	111.19
2	B	701	MMV	O15-C14-C13	2.55	117.69	108.30
3	A	702	NDP	N3A-C2A-N1A	-2.50	125.28	128.67
3	B	702	NDP	C3D-C2D-C1D	-2.50	96.73	101.46
2	A	701	MMV	C10-C9-C5	-2.44	108.00	114.59
3	B	702	NDP	N3A-C2A-N1A	-2.40	125.42	128.67
3	B	702	NDP	C2D-C3D-C4D	2.29	107.04	102.61
3	B	702	NDP	O2A-PA-O1A	2.25	122.93	112.44
3	A	702	NDP	O3B-C3B-C4B	2.20	117.39	111.08
3	A	702	NDP	O2A-PA-O1A	2.17	122.52	112.44
3	A	702	NDP	C2D-C3D-C4D	2.15	106.76	102.61
3	A	702	NDP	C2B-C1B-N9A	2.08	117.19	112.56
3	A	702	NDP	O2N-PN-O1N	2.08	122.13	112.44
3	B	702	NDP	O4B-C1B-C2B	2.06	110.11	106.61
3	B	702	NDP	O2N-PN-O1N	2.02	121.84	112.44
2	B	701	MMV	C23-C22-C17	2.02	118.21	112.71

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	MMV	C12-C13-C14-O15
3	A	702	NDP	PA-O3-PN-O5D
2	A	701	MMV	O11-C12-C13-C14
2	B	701	MMV	C12-C13-C14-O15
3	A	702	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	O4D-C1D-N1N-C2N
3	A	702	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	C2N-C3N-C7N-N7N
2	B	701	MMV	C22-C23-C24-O25
2	B	701	MMV	C22-C23-C24-O26
3	B	702	NDP	C2D-C1D-N1N-C2N
3	A	702	NDP	C2D-C1D-N1N-C2N
2	B	701	MMV	N4-C5-C9-C10

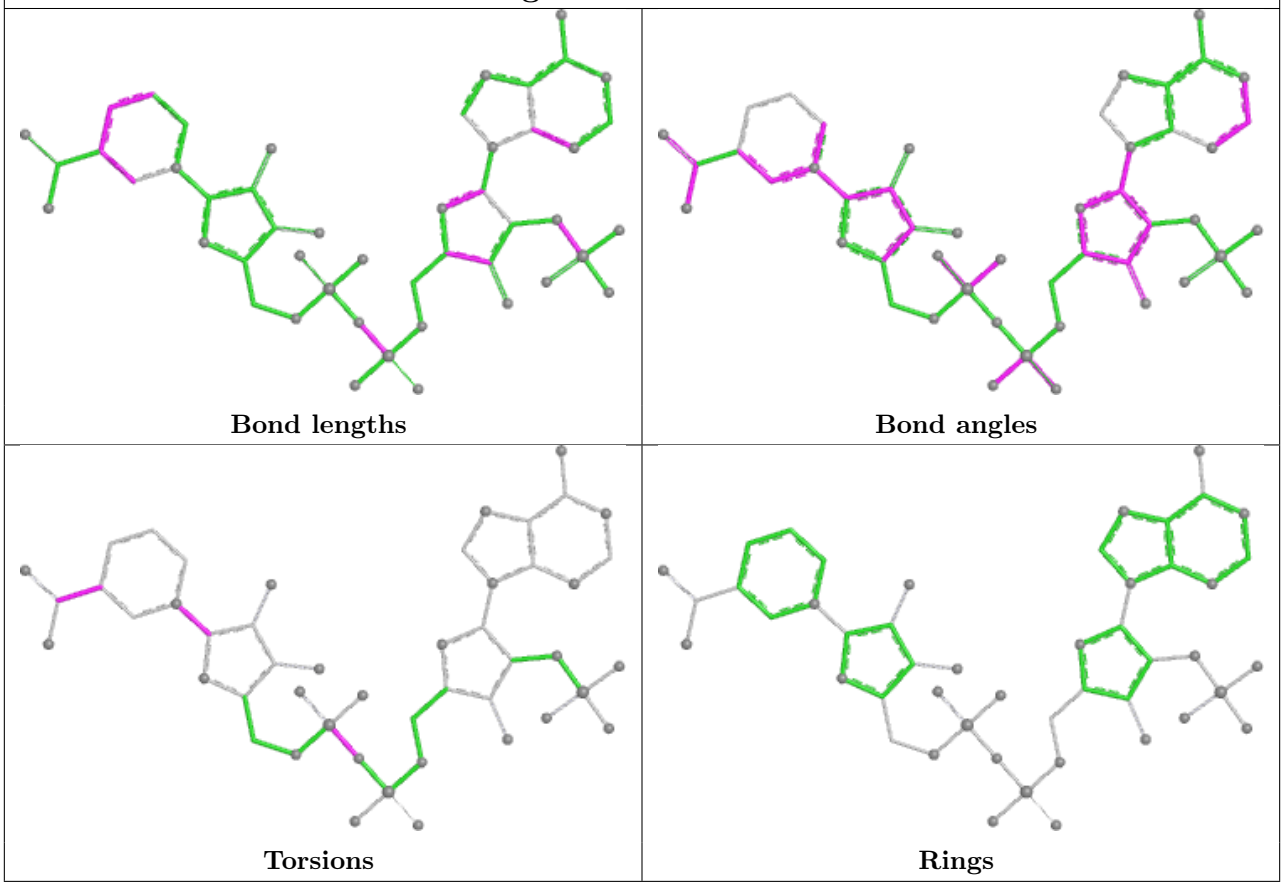
There are no ring outliers.

4 monomers are involved in 10 short contacts:

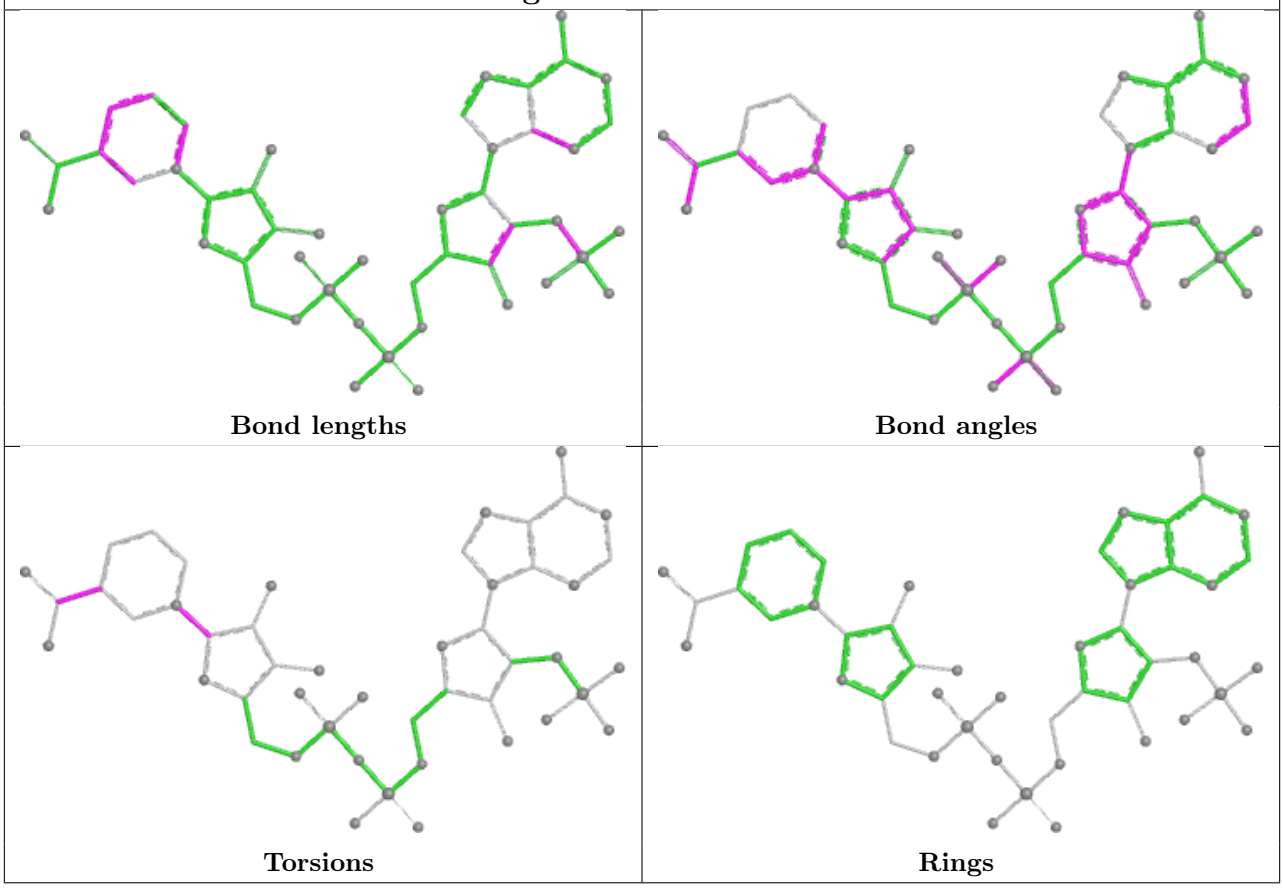
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	NDP	3	0
4	B	703	PO4	1	0
3	B	702	NDP	5	0
2	A	701	MMV	1	0

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.

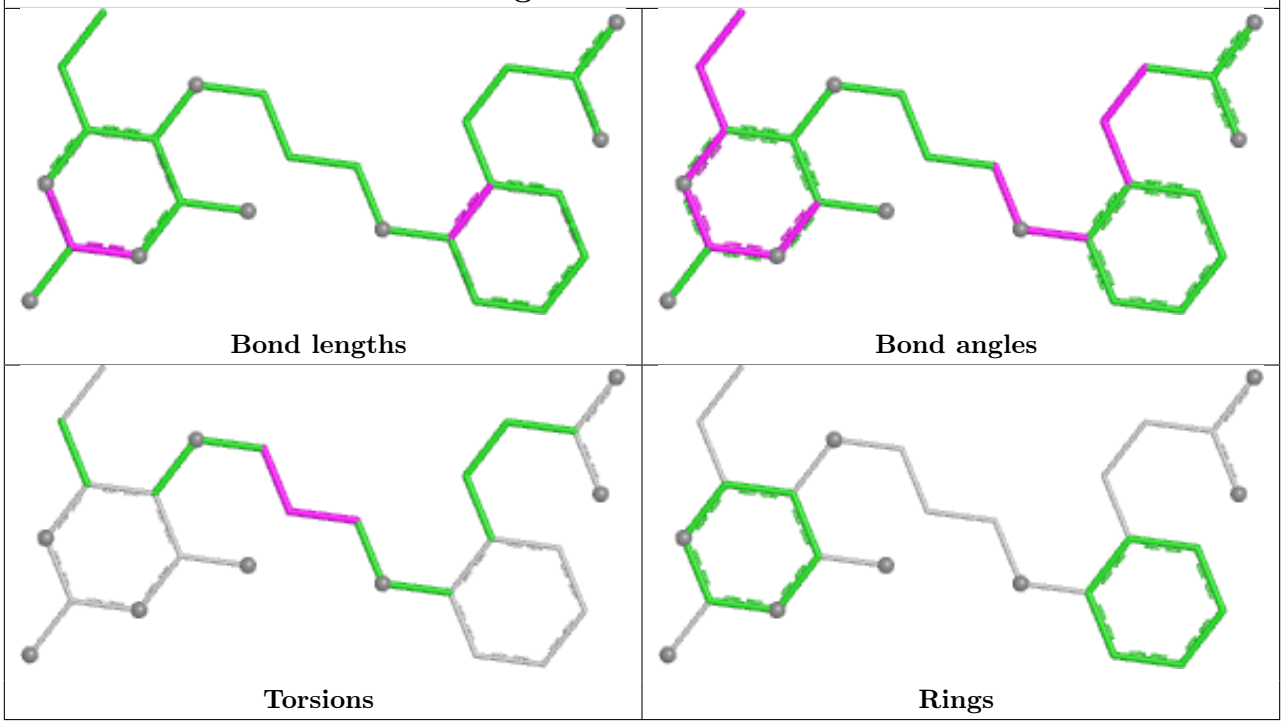
Ligand NDP A 702

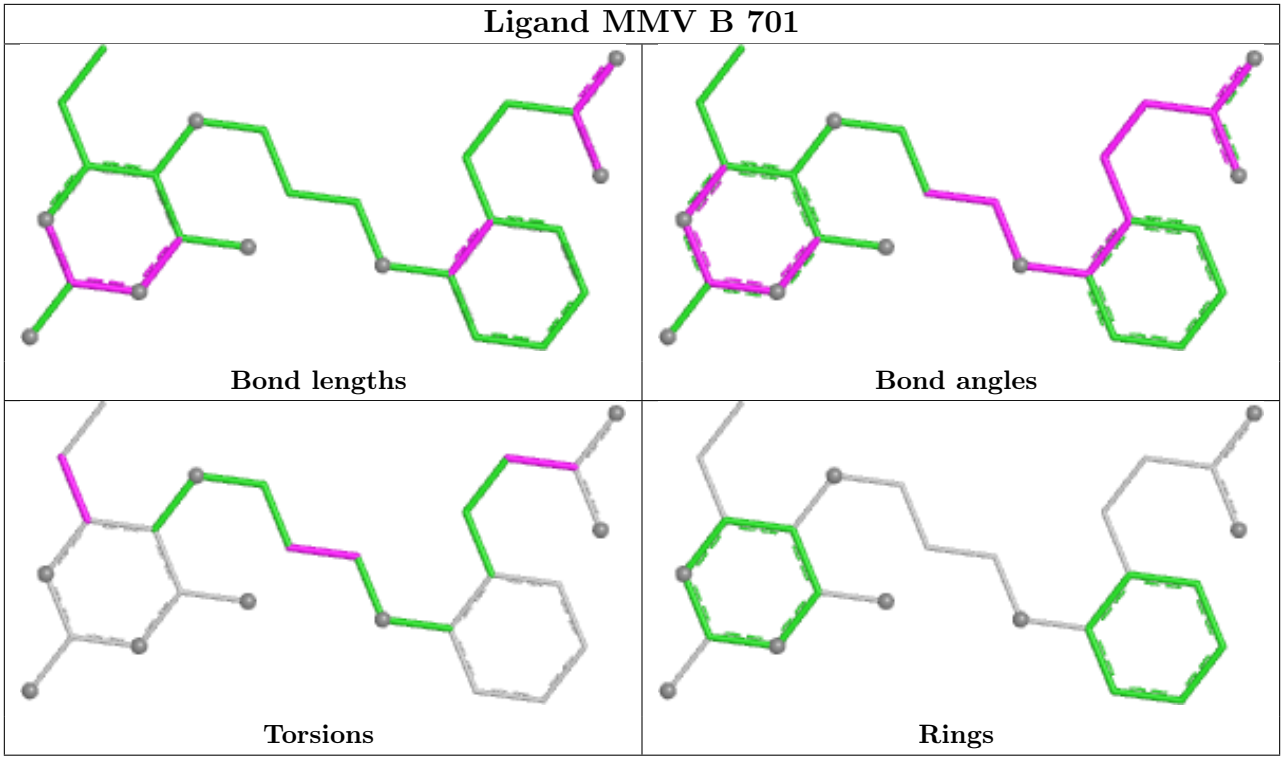


Ligand NDP B 702



Ligand MMV A 701





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	545/608 (89%)	0.08	40 (7%)	15	13	22, 37, 92, 120	0
1	B	544/608 (89%)	0.39	67 (12%)	4	3	22, 43, 104, 121	0
All	All	1089/1216 (89%)	0.23	107 (9%)	7	7	22, 40, 99, 121	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	GLU	9.4
1	B	303	ASN	9.1
1	B	26	GLY	9.0
1	A	24	ASN	8.7
1	B	301	GLU	8.3
1	A	2	MET	8.3
1	B	1	MET	8.1
1	A	283	ASP	7.3
1	B	94	ASN	7.2
1	A	606	MET	7.1
1	B	231	ASN	6.9
1	A	26	GLY	6.7
1	B	27	LYS	6.5
1	A	85	THR	6.5
1	A	301	GLU	6.5
1	A	23	LYS	6.3
1	B	75	TYR	6.2
1	A	1	MET	6.2
1	B	2	MET	6.0
1	B	345	ARG	5.9
1	A	230	ASN	5.9
1	B	25	GLU	5.9
1	B	300	GLU	5.9
1	B	299	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	138	GLU	5.7
1	A	299	LYS	5.6
1	B	95	SER	5.6
1	A	303	ASN	5.6
1	B	346	THR	5.5
1	A	231	ASN	5.4
1	A	345	ARG	5.2
1	A	25	GLU	4.9
1	A	28	LYS	4.9
1	B	230	ASN	4.9
1	B	24	ASN	4.8
1	A	346	THR	4.6
1	B	302	LYS	4.6
1	B	298	GLU	4.5
1	A	29	ASN	4.3
1	B	23	LYS	4.2
1	B	81	LEU	4.2
1	B	135	ASP	4.1
1	A	302	LYS	4.1
1	B	82	ASN	4.1
1	A	284	ASP	4.0
1	A	96	LYS	4.0
1	B	96	LYS	3.9
1	B	136	PHE	3.9
1	B	29	ASN	3.8
1	B	130	THR	3.8
1	B	83	LYS	3.7
1	B	28	LYS	3.7
1	A	605	ASP	3.7
1	B	203	ASN	3.6
1	B	4	GLN	3.6
1	B	605	ASP	3.5
1	B	118	PRO	3.5
1	B	134	GLU	3.3
1	B	283	ASP	3.3
1	A	22	SER	3.3
1	B	22	SER	3.2
1	B	126	ILE	3.2
1	A	307	ILE	3.1
1	A	49	LYS	3.1
1	B	144	ASN	3.1
1	B	3	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	306	SER	3.0
1	A	75	TYR	2.9
1	A	347	GLY	2.9
1	B	305	ASN	2.9
1	A	306	SER	2.8
1	A	97	LYS	2.8
1	B	284	ASP	2.8
1	B	97	LYS	2.7
1	B	125	VAL	2.7
1	B	110	GLU	2.7
1	B	103	VAL	2.7
1	B	43	LYS	2.6
1	B	310	ASN	2.6
1	A	298	GLU	2.6
1	B	603	SER	2.6
1	B	114	LYS	2.6
1	A	286	GLU	2.5
1	B	165	GLY	2.5
1	A	304	LYS	2.5
1	A	297	LYS	2.5
1	B	115	LYS	2.4
1	A	84	GLU	2.4
1	B	139	ASP	2.4
1	A	287	GLU	2.4
1	B	104	MET	2.4
1	B	309	PRO	2.4
1	A	27	LYS	2.3
1	B	307	ILE	2.3
1	B	164	LEU	2.3
1	B	35	TYR	2.3
1	B	343	SER	2.3
1	B	132	LYS	2.3
1	B	347	GLY	2.3
1	B	116	PHE	2.3
1	A	72	LYS	2.2
1	B	129	ARG	2.2
1	B	127	LEU	2.1
1	B	105	GLY	2.1
1	B	297	LYS	2.1
1	A	71	GLU	2.0
1	A	348	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

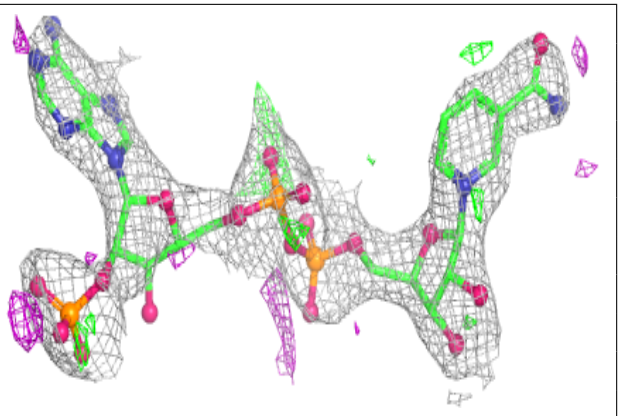
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

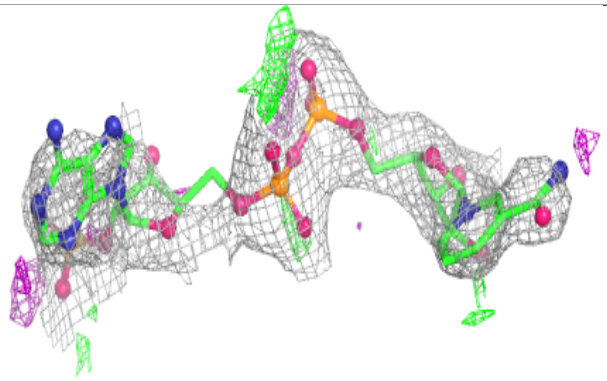
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NDP	B	702	48/48	0.82	0.23	75,86,105,105	0
2	MMV	B	701	26/26	0.89	0.19	56,60,62,64	0
2	MMV	A	701	26/26	0.95	0.14	30,32,36,39	0
3	NDP	A	702	48/48	0.96	0.11	38,44,51,52	0
4	PO4	A	703	5/5	0.96	0.17	53,56,58,59	0
4	PO4	B	703	5/5	0.97	0.15	45,49,52,53	0

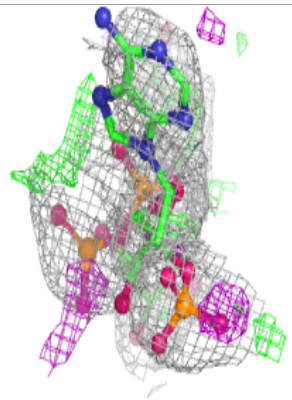
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP B 702:

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

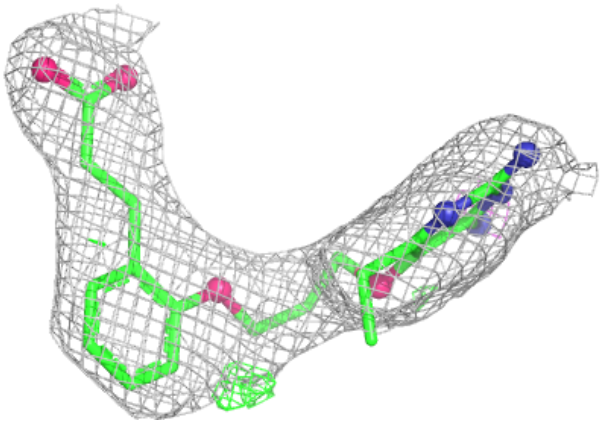


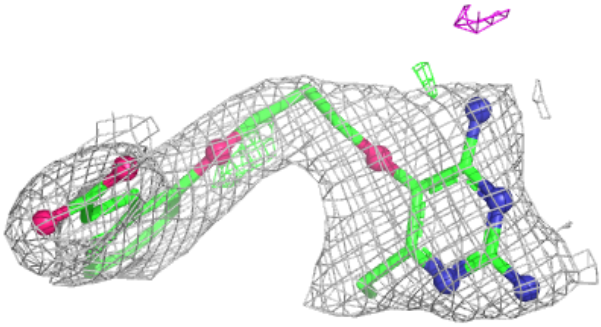


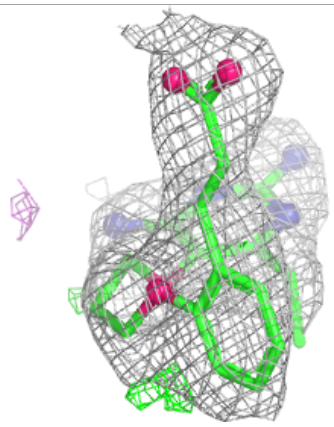


Electron density around MMV B 701:

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

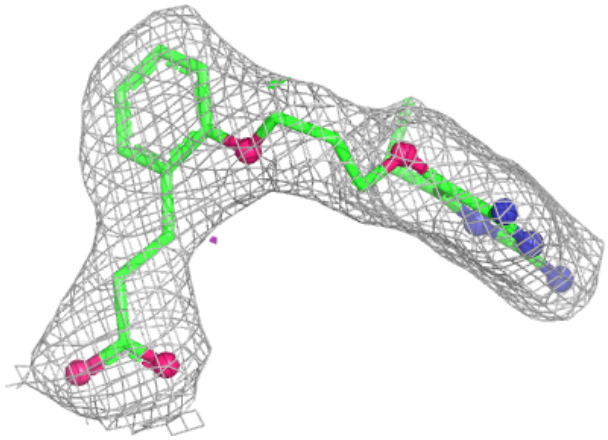


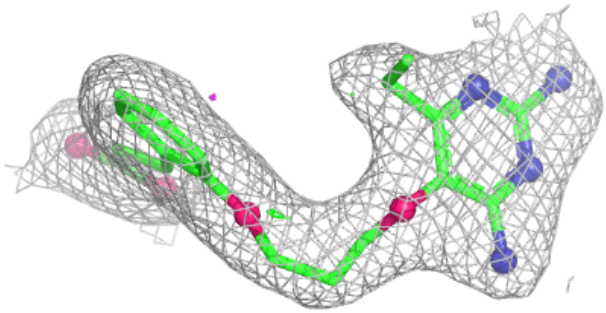


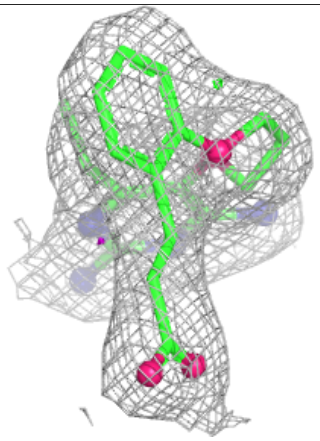


Electron density around MMV A 701:

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

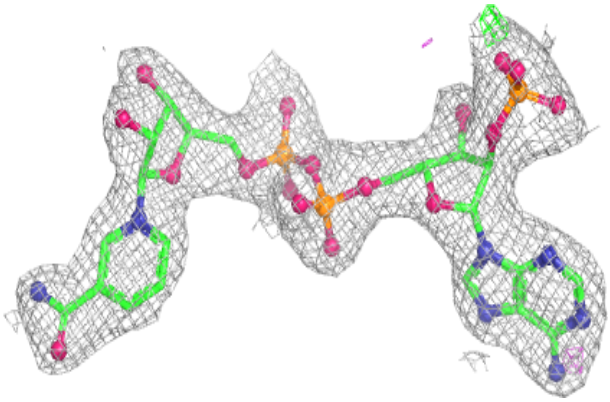


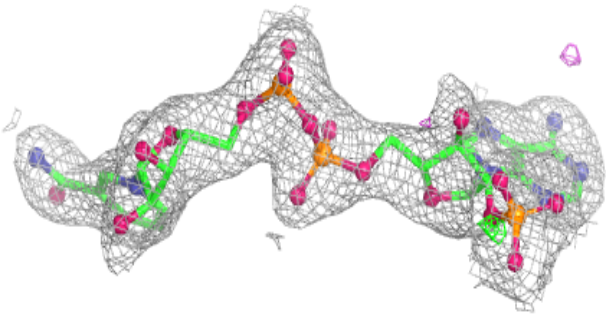


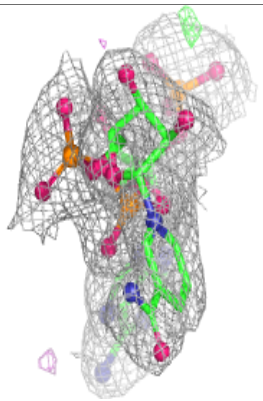


Electron density around NDP A 702:

$2mF_o$-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.