Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:34 PM JST

PDB ID	:	6J1U
Title	:	influenza virus nucleoprotein with a specific inhibitor
Authors	:	Pang, B.; Zhang, W.Z.; Zhang, H.M.; Hao, Q.
Deposited on	:	2018-12-29
Resolution	:	2.80 Å(reported)

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

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

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

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

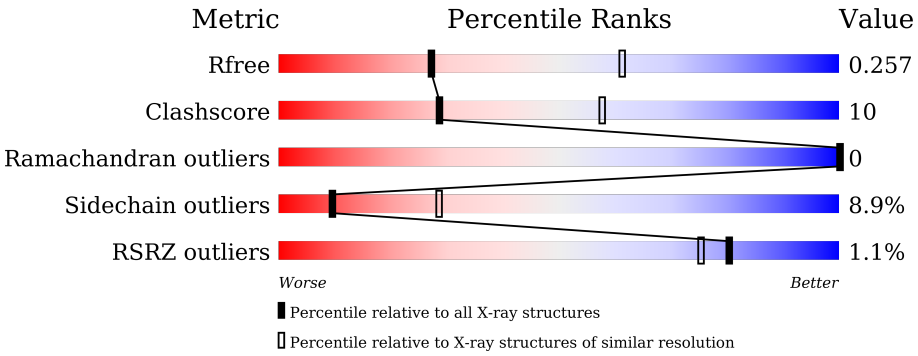
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	498	% 66% 19% • 12%
1	B	498	66% 18% • 12%
1	C	498	2% 67% 19% • 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	B7O	A	501	-	-	-	X
2	B7O	A	502	-	-	-	X
2	B7O	C	501	-	-	-	X

2 Entry composition

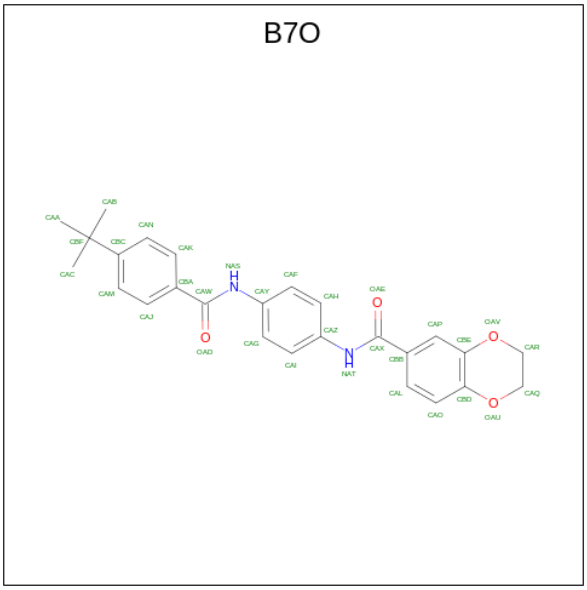
There are 2 unique types of molecules in this entry. The entry contains 10439 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3439	2137	637	640	25			
1	B	437	Total	C	N	O	S	0	0	0
			3436	2136	635	639	26			
1	C	442	Total	C	N	O	S	0	0	0
			3468	2155	645	643	25			

- Molecule 2 is {N}-[4-[(4- {tert}-butylphenyl)carbonylamino]phenyl]-2,3-dihydro-1,4-benzodioxine-6-carboxamide (three-letter code: B7O) (formula: $C_{26}H_{26}N_2O_4$).



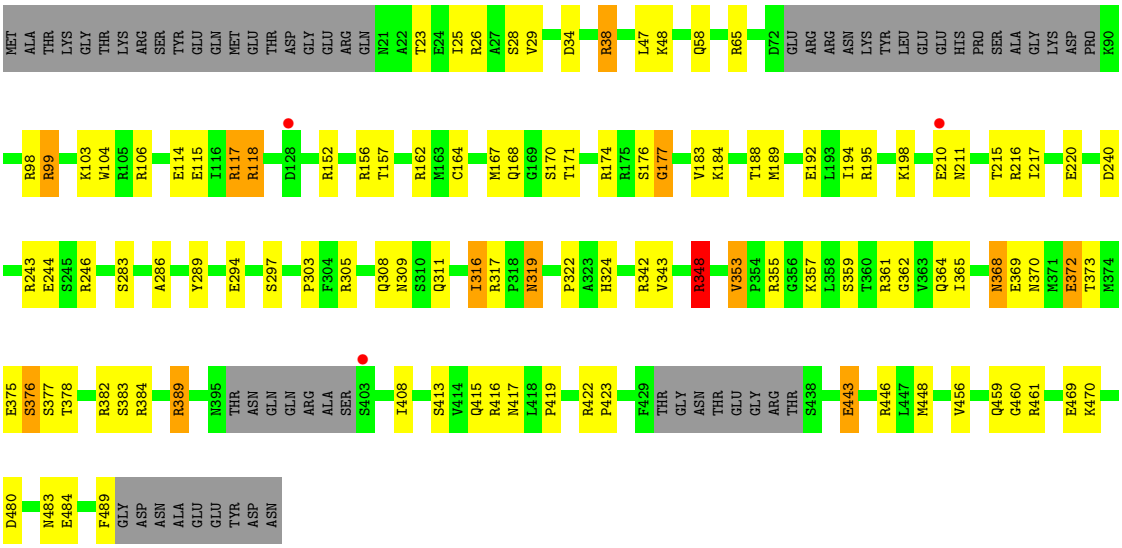
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	26	2	4		
2	A	1	Total	C	N	O	0	0
			32	26	2	4		
2	C	1	Total	C	N	O	0	0
			32	26	2	4		

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.

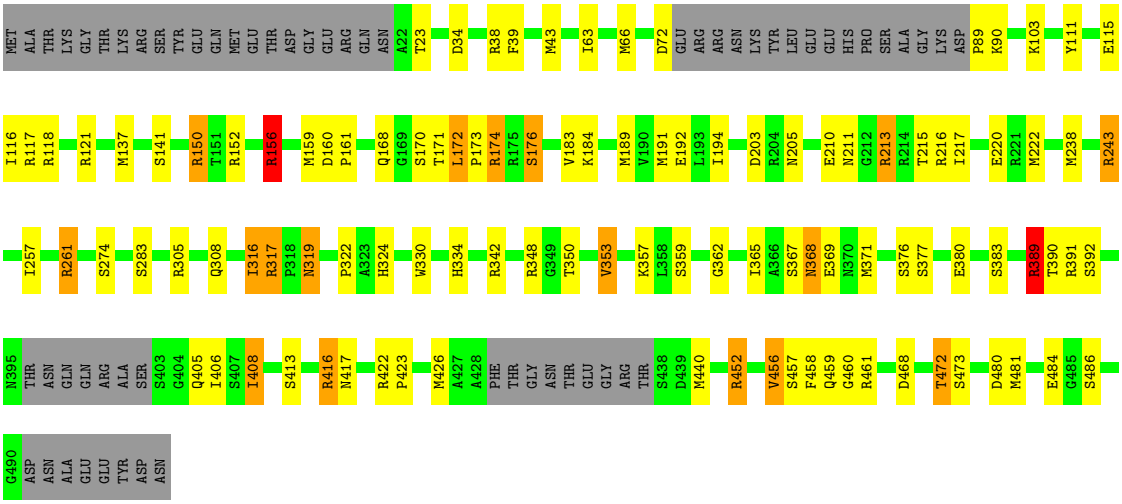
• Molecule 1: Nucleoprotein

Chain A:



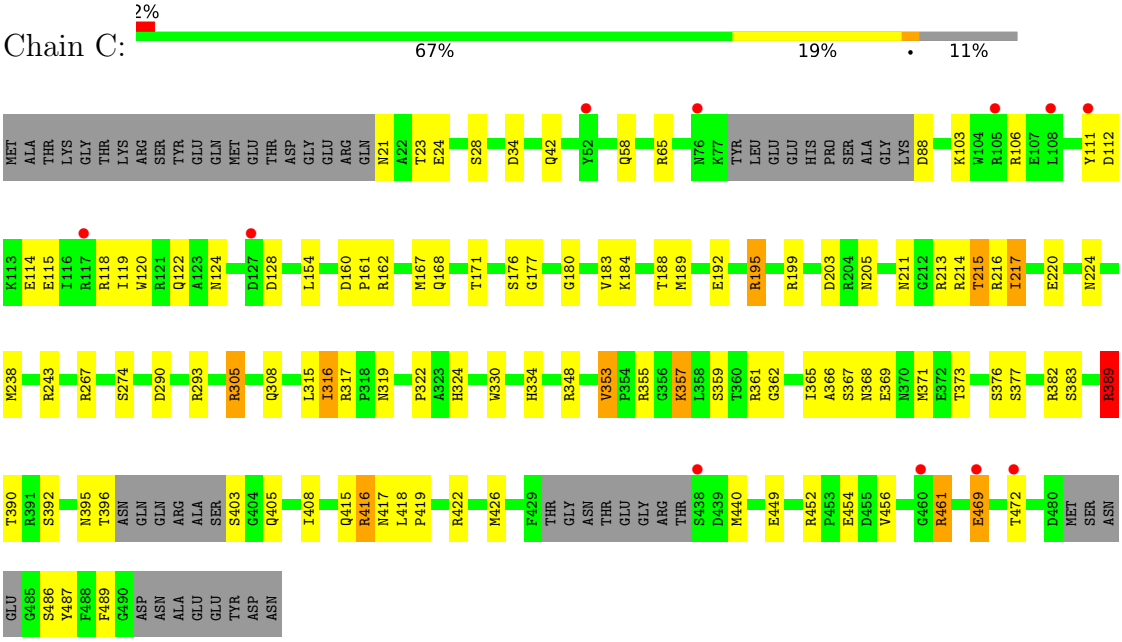
• Molecule 1: Nucleoprotein

Chain B:



• Molecule 1: Nucleoprotein

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.59Å 126.75Å 194.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.53 – 2.80 43.49 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (43.53-2.80) 96.8 (43.49-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.191 , 0.260 0.190 , 0.257	Depositor DCC
R_{free} test set	1810 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10439	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B7O

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	0.71	0/3497	0.82	0/4705
1	B	0.68	0/3494	0.83	2/4698 (0.0%)
1	C	0.60	0/3526	0.79	3/4744 (0.1%)
All	All	0.67	0/10517	0.81	5/14147 (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
1	A	0	14
1	B	0	15
1	C	0	8
All	All	0	37

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	389	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	C	389	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	216	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	389	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	B	342	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ARG	Sidechain
1	A	117	ARG	Sidechain
1	A	118	ARG	Sidechain
1	A	156	ARG	Sidechain
1	A	177	GLY	Peptide
1	A	26	ARG	Sidechain
1	A	348	ARG	Sidechain
1	A	355	ARG	Sidechain
1	A	38	ARG	Sidechain
1	A	384	ARG	Sidechain
1	A	389	ARG	Sidechain
1	A	446	ARG	Sidechain
1	A	461	ARG	Sidechain
1	A	99	ARG	Sidechain
1	B	117	ARG	Sidechain
1	B	121	ARG	Sidechain
1	B	150	ARG	Sidechain
1	B	152	ARG	Sidechain
1	B	156	ARG	Sidechain
1	B	174	ARG	Sidechain
1	B	243	ARG	Sidechain
1	B	261	ARG	Sidechain
1	B	305	ARG	Sidechain
1	B	317	ARG	Sidechain
1	B	38	ARG	Sidechain
1	B	389	ARG	Sidechain
1	B	416	ARG	Sidechain
1	B	452	ARG	Sidechain
1	B	461	ARG	Sidechain
1	C	177	GLY	Peptide
1	C	195	ARG	Sidechain
1	C	199	ARG	Sidechain
1	C	305	ARG	Sidechain
1	C	355	ARG	Sidechain
1	C	389	ARG	Sidechain
1	C	461	ARG	Sidechain
1	C	88	ASP	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	3439	0	3401	70	0
1	B	3436	0	3415	77	0
1	C	3468	0	3425	74	0
2	A	64	0	0	9	0
2	C	32	0	0	8	0
All	All	10439	0	10241	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (201) 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:456:VAL:HG12	1:B:481:MET:CE	1.83	1.09
1:C:224:ASN:HD21	2:C:501:B7O:CAF	1.66	1.09
1:C:21:ASN:HA	1:C:24:GLU:HG3	1.27	1.08
1:C:224:ASN:ND2	2:C:501:B7O:CAF	2.21	1.03
1:B:456:VAL:HG12	1:B:481:MET:HE2	1.00	0.97
1:C:290:ASP:OD2	1:C:293:ARG:NH1	2.01	0.92
1:B:456:VAL:CG1	1:B:481:MET:HE2	1.96	0.91
1:B:308:GLN:HE22	1:B:383:SER:H	1.23	0.86
1:A:308:GLN:HE22	1:A:383:SER:H	1.24	0.85
1:A:317:ARG:HD3	1:A:369:GLU:OE1	1.77	0.83
1:C:308:GLN:HE22	1:C:383:SER:H	1.27	0.83
1:B:324:HIS:HD2	1:B:359:SER:H	1.25	0.82
1:C:324:HIS:HD2	1:C:359:SER:H	1.24	0.82
1:A:460:GLY:H	1:C:415:GLN:NE2	1.78	0.82
1:C:154:LEU:HD21	1:C:167:MET:HE3	1.61	0.81
1:A:305:ARG:HD2	2:A:501:B7O:CAB	2.12	0.80
1:C:224:ASN:HD21	2:C:501:B7O:CAH	1.95	0.79
1:A:240:ASP:OD1	1:A:243:ARG:NH1	2.16	0.79
1:B:39:PHE:CZ	1:B:43:MET:HE3	2.19	0.77
1:C:211:ASN:O	1:C:215:THR:HG23	1.84	0.77
1:A:460:GLY:H	1:C:415:GLN:HE21	1.32	0.76
1:C:224:ASN:ND2	2:C:501:B7O:CAH	2.49	0.76
1:B:39:PHE:CE1	1:B:43:MET:CE	2.72	0.73
1:A:311:GLN:OE1	1:A:378:THR:HG23	1.89	0.73
1:A:324:HIS:HD2	1:A:359:SER:H	1.35	0.72
1:B:159:MET:HE1	1:B:191:MET:HB2	1.72	0.72
2:C:501:B7O:CAF	2:C:501:B7O:CAJ	2.67	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLN:HE21	1:B:460:GLY:H	1.34	0.71
1:B:317:ARG:HD3	1:B:369:GLU:OE1	1.90	0.71
1:B:368:ASN:HD22	1:B:368:ASN:H	1.40	0.70
1:C:324:HIS:CD2	1:C:359:SER:H	2.08	0.70
1:A:342:ARG:HH22	1:C:417:ASN:HD21	1.40	0.69
1:B:192:GLU:HB3	1:B:222:MET:CE	2.22	0.69
1:C:305:ARG:HH22	1:C:469:GLU:HG3	1.59	0.68
1:A:417:ASN:HB3	1:B:481:MET:HE3	1.75	0.68
1:B:203:ASP:OD1	1:B:205:ASN:OD1	2.12	0.67
1:C:184:LYS:HD3	1:C:189:MET:HE3	1.77	0.66
1:A:343:VAL:HG21	1:C:416:ARG:NH1	2.11	0.66
1:B:317:ARG:NH2	1:B:362:GLY:O	2.28	0.66
1:C:449:GLU:O	1:C:452:ARG:NH1	2.28	0.66
1:B:39:PHE:CE1	1:B:43:MET:HE3	2.31	0.66
1:B:66:MET:HE3	1:B:116:ILE:HD11	1.79	0.65
1:B:156:ARG:HH21	1:B:156:ARG:HG2	1.61	0.65
1:C:220:GLU:HG2	1:C:243:ARG:HG3	1.79	0.64
1:A:415:GLN:NE2	1:B:460:GLY:H	1.95	0.64
1:A:324:HIS:CD2	1:A:359:SER:H	2.13	0.64
1:B:472:THR:HG22	1:B:473:SER:OG	1.98	0.64
1:A:162:ARG:CG	1:C:403:SER:HA	2.29	0.63
1:B:348:ARG:HA	1:B:383:SER:HB2	1.80	0.63
1:B:156:ARG:HG2	1:B:156:ARG:NH2	2.13	0.62
1:B:211:ASN:O	1:B:215:THR:HG23	2.00	0.62
1:C:21:ASN:CA	1:C:24:GLU:HG3	2.17	0.62
1:A:114:GLU:HA	1:A:117:ARG:HH21	1.64	0.62
1:C:168:GLN:HG2	1:C:183:VAL:O	1.99	0.62
1:B:184:LYS:HD3	1:B:189:MET:CE	2.29	0.61
1:B:324:HIS:CD2	1:B:359:SER:H	2.12	0.61
1:B:408:ILE:HD13	1:C:487:TYR:HD1	1.65	0.61
1:A:184:LYS:HD3	1:A:189:MET:HE3	1.83	0.61
1:A:211:ASN:O	1:A:215:THR:HG23	2.00	0.61
1:A:103:LYS:HE2	1:A:372:GLU:HG3	1.83	0.61
1:A:305:ARG:HB3	2:A:501:B7O:CAB	2.31	0.61
1:C:408:ILE:HD11	1:C:418:LEU:HD22	1.83	0.60
1:A:489:PHE:H	1:C:405:GLN:NE2	1.98	0.60
1:C:317:ARG:NH2	1:C:362:GLY:O	2.34	0.60
1:C:317:ARG:HD3	1:C:369:GLU:OE1	2.01	0.60
1:B:137:MET:HE1	1:B:176:SER:HB3	1.83	0.60
1:B:160:ASP:OD1	1:B:161:PRO:HD2	2.01	0.60
1:C:348:ARG:HA	1:C:383:SER:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:SER:HB3	1:C:180:GLY:HA3	1.84	0.59
1:B:168:GLN:HG2	1:B:183:VAL:O	2.01	0.59
1:B:390:THR:HB	1:B:392:SER:H	1.67	0.59
1:A:184:LYS:HD3	1:A:189:MET:CE	2.33	0.59
1:A:168:GLN:HG2	1:A:183:VAL:O	2.04	0.58
2:C:501:B7O:CAH	2:C:501:B7O:OAE	2.52	0.58
1:A:34:ASP:OD1	1:A:38:ARG:NH1	2.36	0.58
1:B:216:ARG:NH2	1:B:243:ARG:O	2.37	0.58
1:B:192:GLU:HB3	1:B:222:MET:HE3	1.86	0.57
1:A:58:GLN:HG2	1:A:365:ILE:HD12	1.87	0.57
1:C:184:LYS:HD3	1:C:189:MET:CE	2.35	0.56
1:B:413:SER:HB2	1:C:390:THR:HG23	1.86	0.56
2:A:502:B7O:CAK	2:A:502:B7O:CAF	2.84	0.56
1:A:448:MET:HB3	1:C:426:MET:HE3	1.88	0.56
2:A:501:B7O:CAG	2:A:501:B7O:CBA	2.82	0.56
1:A:317:ARG:NH2	1:A:362:GLY:O	2.36	0.56
2:A:501:B7O:CAG	2:A:501:B7O:CAJ	2.83	0.56
1:C:308:GLN:HA	1:C:382:ARG:HG2	1.88	0.56
1:A:176:SER:OG	1:A:177:GLY:N	2.39	0.55
1:B:405:GLN:NE2	1:C:489:PHE:H	2.04	0.55
1:B:456:VAL:CG1	1:B:481:MET:CE	2.68	0.55
1:C:115:GLU:OE1	1:C:118:ARG:NH1	2.39	0.55
1:A:47:LEU:O	1:A:98:ARG:NH2	2.25	0.55
1:C:308:GLN:HE22	1:C:383:SER:N	1.99	0.55
1:B:66:MET:CE	1:B:116:ILE:HD11	2.37	0.55
1:A:443:GLU:OE2	1:A:443:GLU:HA	2.07	0.55
1:B:408:ILE:O	1:C:267:ARG:HD3	2.07	0.55
1:B:150:ARG:NH2	1:B:170:SER:OG	2.41	0.54
1:B:408:ILE:HD13	1:C:487:TYR:CD1	2.43	0.53
1:C:106:ARG:HH21	1:C:365:ILE:HG22	1.72	0.53
1:A:220:GLU:HG2	1:A:243:ARG:HG3	1.91	0.53
1:B:406:ILE:HD13	1:C:162:ARG:HB3	1.91	0.53
1:A:162:ARG:HG3	1:C:403:SER:HA	1.89	0.53
1:C:106:ARG:HB3	1:C:371:MET:HG3	1.89	0.53
1:A:174:ARG:NH1	1:A:192:GLU:O	2.41	0.53
1:C:154:LEU:HD21	1:C:167:MET:CE	2.37	0.53
1:B:115:GLU:OE1	1:B:118:ARG:NH1	2.42	0.52
1:B:330:TRP:CE2	1:B:348:ARG:HG3	2.44	0.52
1:C:390:THR:HB	1:C:392:SER:H	1.74	0.52
1:A:289:TYR:OH	1:A:294:GLU:HG2	2.08	0.52
1:B:210:GLU:O	1:B:213:ARG:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:GLU:OE1	1:A:118:ARG:NH1	2.42	0.51
1:A:174:ARG:HH12	1:A:195:ARG:HB2	1.75	0.51
1:A:460:GLY:N	1:C:415:GLN:HE21	2.06	0.51
1:B:274:SER:OG	1:B:334:HIS:HD2	1.94	0.51
1:A:308:GLN:HE22	1:A:383:SER:N	2.02	0.51
1:A:419:PRO:HB3	1:B:484:GLU:HA	1.93	0.51
1:C:176:SER:CB	1:C:180:GLY:HA3	2.40	0.51
1:C:238:MET:HG3	1:C:440:MET:HB3	1.92	0.51
1:A:114:GLU:CA	1:A:117:ARG:HH21	2.23	0.51
1:B:184:LYS:HD3	1:B:189:MET:HE3	1.92	0.50
1:A:370:ASN:ND2	1:A:373:THR:HG23	2.27	0.49
1:A:162:ARG:HG2	1:C:403:SER:HA	1.95	0.49
1:B:220:GLU:HG2	1:B:243:ARG:HG3	1.95	0.49
1:A:114:GLU:HG3	1:A:117:ARG:NH2	2.28	0.49
1:B:324:HIS:HD2	1:B:359:SER:N	2.04	0.48
1:B:365:ILE:HG21	1:B:371:MET:HE1	1.96	0.48
1:C:330:TRP:CE2	1:C:348:ARG:HG3	2.48	0.48
1:A:220:GLU:HG2	1:A:243:ARG:CG	2.44	0.48
1:A:342:ARG:HH22	1:C:417:ASN:ND2	2.07	0.48
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.41	0.48
1:B:159:MET:CE	1:B:191:MET:HB2	2.41	0.48
1:B:348:ARG:NH2	1:B:380:GLU:O	2.46	0.47
1:C:58:GLN:HG2	1:C:365:ILE:HD12	1.95	0.47
1:B:417:ASN:HD22	1:B:417:ASN:H	1.61	0.47
1:B:371:MET:HA	1:B:371:MET:HE2	1.97	0.47
1:B:408:ILE:HD12	1:B:408:ILE:HA	1.74	0.47
1:B:89:PRO:HB2	1:B:90:LYS:H	1.61	0.46
1:C:211:ASN:O	1:C:215:THR:CG2	2.58	0.46
1:A:348:ARG:HA	1:A:383:SER:HB2	1.96	0.46
1:C:214:ARG:HA	1:C:217:ILE:HG22	1.98	0.46
1:A:316:ILE:HD13	1:A:322:PRO:HG3	1.97	0.45
1:A:368:ASN:ND2	1:A:368:ASN:H	2.14	0.45
1:B:422:ARG:HB3	1:B:423:PRO:HD3	1.98	0.45
1:C:160:ASP:OD1	1:C:161:PRO:HD2	2.16	0.45
1:A:317:ARG:NH1	1:A:369:GLU:OE2	2.49	0.45
1:B:194:ILE:HD11	1:B:257:ILE:HD12	1.99	0.45
1:B:220:GLU:HG2	1:B:243:ARG:CG	2.46	0.45
1:B:160:ASP:OD2	1:B:261:ARG:NH1	2.49	0.45
1:C:417:ASN:HD22	1:C:417:ASN:H	1.63	0.45
1:B:184:LYS:HD3	1:B:189:MET:HE1	1.99	0.45
1:C:353:VAL:HG13	1:C:357:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLU:H	1:A:210:GLU:CD	2.20	0.44
1:B:468:ASP:OD1	1:B:472:THR:HB	2.18	0.44
1:A:456:VAL:HG22	1:A:459:GLN:NE2	2.33	0.44
1:A:489:PHE:HB2	1:C:405:GLN:HE21	1.82	0.44
1:B:137:MET:CE	1:B:173:PRO:HG2	2.47	0.44
1:C:316:ILE:HD13	1:C:322:PRO:HG3	1.99	0.44
1:A:164:CYS:HA	1:A:167:MET:HG2	2.00	0.44
1:A:422:ARG:HB3	1:A:423:PRO:HD3	1.98	0.44
1:C:192:GLU:HG2	1:C:195:ARG:HH12	1.82	0.44
1:C:308:GLN:NE2	1:C:383:SER:H	2.06	0.44
1:C:220:GLU:HG2	1:C:243:ARG:CG	2.47	0.43
1:B:316:ILE:HD13	1:B:322:PRO:HG3	2.00	0.43
1:A:308:GLN:HA	1:A:382:ARG:HG2	1.99	0.43
1:B:317:ARG:NH1	1:B:369:GLU:OE2	2.51	0.43
1:B:371:MET:HA	1:B:371:MET:CE	2.48	0.43
1:A:413:SER:HB2	1:B:390:THR:HG23	2.01	0.43
2:A:502:B7O:CAF	2:A:502:B7O:CBA	2.97	0.43
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.38	0.43
1:A:353:VAL:HG13	1:A:357:LYS:HB2	2.00	0.43
2:C:501:B7O:CAF	2:C:501:B7O:CBA	2.95	0.43
1:A:157:THR:HG22	1:A:194:ILE:HG21	2.01	0.43
1:A:470:LYS:HA	1:A:470:LYS:HD3	1.81	0.43
1:A:448:MET:HE1	1:C:426:MET:HE1	2.01	0.42
1:B:426:MET:HB3	1:B:452:ARG:CZ	2.49	0.42
1:C:120:TRP:CE2	1:C:124:ASN:ND2	2.87	0.42
1:C:315:LEU:HD12	1:C:365:ILE:HD13	2.00	0.42
1:B:353:VAL:HG13	1:B:357:LYS:HB3	2.01	0.42
1:B:43:MET:HG2	1:B:63:ILE:HG23	2.00	0.42
1:B:141:SER:HB2	1:B:172:LEU:HD13	2.02	0.42
1:A:309:ASN:HB2	2:A:501:B7O:CAJ	2.49	0.42
1:C:184:LYS:HG2	1:C:188:THR:HG21	2.02	0.42
1:A:415:GLN:HB2	1:B:458:PHE:O	2.20	0.42
1:B:405:GLN:HE21	1:C:489:PHE:H	1.66	0.42
1:A:25:ILE:O	1:A:29:VAL:HG13	2.19	0.42
1:B:238:MET:HG3	1:B:440:MET:HB3	2.01	0.42
1:C:274:SER:OG	1:C:334:HIS:HD2	2.03	0.42
2:A:502:B7O:CAK	2:A:502:B7O:CAY	2.97	0.41
1:A:216:ARG:NH2	1:A:243:ARG:O	2.53	0.41
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.89	0.41
1:A:286:ALA:O	2:A:502:B7O:CAC	2.68	0.41
1:C:408:ILE:HG12	1:C:419:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:MET:HE1	1:B:173:PRO:HG2	2.02	0.41
1:B:408:ILE:CD1	1:C:487:TYR:HD1	2.33	0.41
1:A:489:PHE:H	1:C:405:GLN:HE21	1.68	0.41
1:C:42:GLN:HG2	1:C:119:ILE:HG23	2.03	0.41
1:A:104:TRP:NE1	1:A:376:SER:HB3	2.36	0.41
1:C:106:ARG:NH2	1:C:366:ALA:O	2.54	0.41
1:A:170:SER:HA	1:A:188:THR:HG23	2.03	0.40
1:C:224:ASN:HD22	2:C:501:B7O:CAJ	2.34	0.40
1:A:297:SER:O	1:A:303:PRO:HD3	2.21	0.40
1:C:114:GLU:O	1:C:118:ARG:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/498 (86%)	420 (98%)	9 (2%)	0	100	100
1	B	429/498 (86%)	419 (98%)	10 (2%)	0	100	100
1	C	432/498 (87%)	420 (97%)	12 (3%)	0	100	100
All	All	1290/1494 (86%)	1259 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	366/422 (87%)	335 (92%)	31 (8%)	10 31
1	B	367/422 (87%)	336 (92%)	31 (8%)	11 31
1	C	367/422 (87%)	331 (90%)	36 (10%)	8 24
All	All	1100/1266 (87%)	1002 (91%)	98 (9%)	9 28

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	THR
1	A	28	SER
1	A	48	LYS
1	A	65	ARG
1	A	99	ARG
1	A	152	ARG
1	A	171	THR
1	A	198	LYS
1	A	217	ILE
1	A	244	GLU
1	A	246	ARG
1	A	283	SER
1	A	316	ILE
1	A	319	ASN
1	A	348	ARG
1	A	353	VAL
1	A	361	ARG
1	A	364	GLN
1	A	368	ASN
1	A	372	GLU
1	A	375	GLU
1	A	376	SER
1	A	377	SER
1	A	389	ARG
1	A	408	ILE
1	A	416	ARG
1	A	443	GLU
1	A	469	GLU
1	A	480	ASP
1	A	483	ASN
1	A	484	GLU
1	B	23	THR
1	B	34	ASP
1	B	72	ASP

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Mol	Chain	Res	Type
1	B	103	LYS
1	B	111	TYR
1	B	156	ARG
1	B	171	THR
1	B	172	LEU
1	B	174	ARG
1	B	176	SER
1	B	213	ARG
1	B	217	ILE
1	B	283	SER
1	B	316	ILE
1	B	319	ASN
1	B	350	THR
1	B	353	VAL
1	B	367	SER
1	B	368	ASN
1	B	376	SER
1	B	377	SER
1	B	389	ARG
1	B	391	ARG
1	B	408	ILE
1	B	416	ARG
1	B	456	VAL
1	B	457	SER
1	B	459	GLN
1	B	472	THR
1	B	480	ASP
1	B	486	SER
1	C	23	THR
1	C	28	SER
1	C	34	ASP
1	C	65	ARG
1	C	103	LYS
1	C	111	TYR
1	C	112	ASP
1	C	122	GLN
1	C	128	ASP
1	C	171	THR
1	C	203	ASP
1	C	205	ASN
1	C	213	ARG
1	C	215	THR

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Mol	Chain	Res	Type
1	C	217	ILE
1	C	316	ILE
1	C	319	ASN
1	C	353	VAL
1	C	357	LYS
1	C	361	ARG
1	C	367	SER
1	C	368	ASN
1	C	373	THR
1	C	376	SER
1	C	377	SER
1	C	389	ARG
1	C	395	ASN
1	C	396	THR
1	C	416	ARG
1	C	422	ARG
1	C	454	GLU
1	C	456	VAL
1	C	461	ARG
1	C	469	GLU
1	C	472	THR
1	C	486	SER

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	211	ASN
1	A	235	GLN
1	A	272	HIS
1	A	308	GLN
1	A	319	ASN
1	A	324	HIS
1	A	334	HIS
1	A	368	ASN
1	A	415	GLN
1	A	483	ASN
1	B	122	GLN
1	B	211	ASN
1	B	235	GLN
1	B	272	HIS
1	B	308	GLN
1	B	319	ASN

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Mol	Chain	Res	Type
1	B	324	HIS
1	B	334	HIS
1	B	368	ASN
1	B	370	ASN
1	B	405	GLN
1	B	417	ASN
1	B	459	GLN
1	C	224	ASN
1	C	235	GLN
1	C	272	HIS
1	C	308	GLN
1	C	324	HIS
1	C	334	HIS
1	C	405	GLN
1	C	415	GLN
1	C	417	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	B7O	C	501	-	35,35,35	1.02	2 (5%)	50,50,50	2.57	18 (36%)
2	B7O	A	502	-	35,35,35	2.27	8 (22%)	50,50,50	1.87	11 (22%)
2	B7O	A	501	-	35,35,35	2.21	6 (17%)	50,50,50	2.26	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B7O	C	501	-	-	4/22/29/29	0/4/4/4
2	B7O	A	502	-	-	3/22/29/29	0/4/4/4
2	B7O	A	501	-	-	6/22/29/29	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	B7O	CBF-CBC	-7.13	1.39	1.53
2	A	502	B7O	CBF-CBC	-6.49	1.40	1.53
2	A	501	B7O	CBB-CAX	-5.55	1.38	1.50
2	A	502	B7O	CAZ-NAT	-5.45	1.30	1.41
2	A	501	B7O	CBA-CAW	-5.36	1.39	1.50
2	A	502	B7O	CBB-CAX	-5.30	1.39	1.50
2	A	501	B7O	CAZ-NAT	-4.88	1.31	1.41
2	A	502	B7O	CBA-CAW	-4.14	1.41	1.50
2	A	502	B7O	OAV-CBE	-3.91	1.33	1.37
2	A	502	B7O	OAU-CBD	-3.65	1.33	1.37
2	A	502	B7O	CAY-NAS	-3.51	1.34	1.41
2	A	502	B7O	OAU-CAQ	-3.38	1.35	1.43
2	C	501	B7O	CAY-NAS	-2.61	1.36	1.41
2	A	501	B7O	CAI-CAZ	-2.51	1.35	1.39
2	A	501	B7O	OAV-CBE	-2.36	1.35	1.37
2	C	501	B7O	CAI-CAG	2.09	1.42	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	B7O	CBA-CAW-NAS	8.80	135.28	115.92
2	A	501	B7O	CAI-CAG-CAY	7.13	128.53	120.30
2	A	502	B7O	OAV-CBE-CBD	-6.46	116.25	122.03
2	A	501	B7O	OAV-CBE-CBD	-6.24	116.44	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	B7O	OAU-CBD-CBE	-5.79	116.84	122.03
2	C	501	B7O	OAD-CAW-CBA	-5.58	110.98	120.94
2	A	501	B7O	CAQ-OAU-CBD	-4.75	105.47	113.65
2	A	502	B7O	CAQ-OAU-CBD	-4.68	105.58	113.65
2	C	501	B7O	CAH-CAF-CAY	4.68	125.70	120.30
2	A	501	B7O	CAF-CAY-CAG	-4.66	112.66	119.03
2	C	501	B7O	OAD-CAW-NAS	-4.44	113.56	123.71
2	C	501	B7O	OAE-CAX-CBB	-4.27	113.33	120.94
2	A	501	B7O	OAU-CBD-CBE	-4.02	118.43	122.03
2	A	502	B7O	OAU-CBD-CBE	-3.97	118.47	122.03
2	A	501	B7O	CAR-OAV-CBE	-3.94	106.86	113.65
2	C	501	B7O	OAU-CBD-CAO	3.89	123.09	116.85
2	A	501	B7O	CAH-CAZ-NAT	3.81	133.22	120.40
2	C	501	B7O	OAV-CBE-CBD	-3.71	118.70	122.03
2	C	501	B7O	CAQ-OAU-CBD	3.70	120.02	113.65
2	C	501	B7O	CBB-CAX-NAT	3.69	124.04	115.92
2	A	501	B7O	CAI-CAZ-NAT	-3.58	108.36	120.40
2	A	502	B7O	CBB-CAX-NAT	-3.26	108.75	115.92
2	A	502	B7O	CAO-CAL-CBB	3.21	124.51	120.78
2	A	501	B7O	OAV-CBE-CAP	3.18	121.94	117.05
2	A	502	B7O	OAV-CBE-CAP	2.73	121.25	117.05
2	C	501	B7O	OAV-CBE-CAP	2.68	121.17	117.05
2	A	502	B7O	CBA-CAW-NAS	2.67	121.80	115.92
2	C	501	B7O	CAG-CAY-NAS	2.60	129.16	120.40
2	A	501	B7O	OAU-CBD-CAO	2.55	120.94	116.85
2	C	501	B7O	CAJ-CBA-CAK	-2.53	114.98	118.59
2	A	501	B7O	OAD-CAW-CBA	-2.48	116.52	120.94
2	C	501	B7O	CAJ-CBA-CAW	2.43	128.49	120.62
2	C	501	B7O	CAF-CAY-CAG	-2.42	115.72	119.03
2	A	502	B7O	CBB-CAP-CBE	-2.39	116.43	119.61
2	A	501	B7O	CBA-CAW-NAS	2.37	121.14	115.92
2	C	501	B7O	CAM-CAJ-CBA	2.34	123.50	120.78
2	A	502	B7O	OAU-CBD-CAO	2.32	120.57	116.85
2	C	501	B7O	CAC-CBF-CAA	2.30	115.80	108.32
2	A	501	B7O	CAG-CAI-CAZ	-2.26	117.69	120.30
2	C	501	B7O	CAH-CAZ-CAI	-2.20	116.02	119.03
2	A	502	B7O	OAE-CAX-NAT	2.06	128.41	123.71
2	A	502	B7O	CAP-CBE-CBD	2.01	122.50	119.84

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	B7O	OAD-CAW-NAS-CAY
2	A	501	B7O	CBA-CAW-NAS-CAY
2	A	501	B7O	OAD-CAW-NAS-CAY
2	A	502	B7O	OAD-CAW-NAS-CAY
2	A	502	B7O	CBA-CAW-NAS-CAY
2	C	501	B7O	CBA-CAW-NAS-CAY
2	A	501	B7O	NAS-CAW-CBA-CAK
2	A	501	B7O	NAS-CAW-CBA-CAJ
2	A	501	B7O	OAD-CAW-CBA-CAK
2	A	501	B7O	OAD-CAW-CBA-CAJ
2	A	502	B7O	NAT-CAX-CBB-CAP
2	C	501	B7O	CAM-CBC-CBF-CAA
2	C	501	B7O	CAN-CBC-CBF-CAA

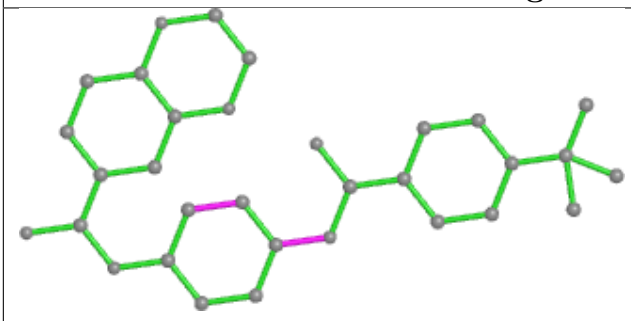
There are no ring outliers.

3 monomers are involved in 17 short contacts:

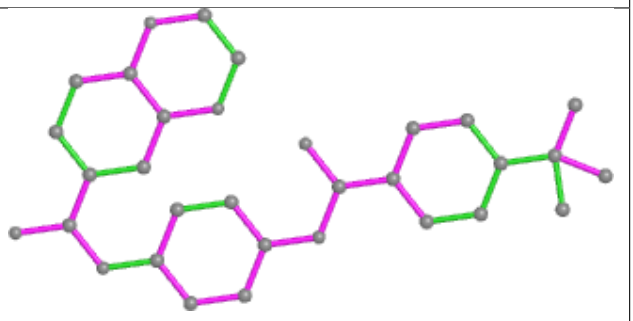
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	B7O	8	0
2	A	502	B7O	4	0
2	A	501	B7O	5	0

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.

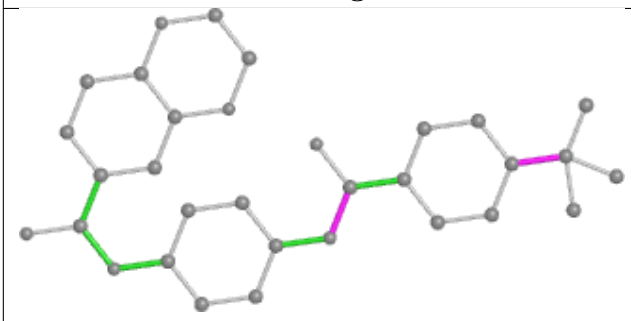
Ligand B7O C 501



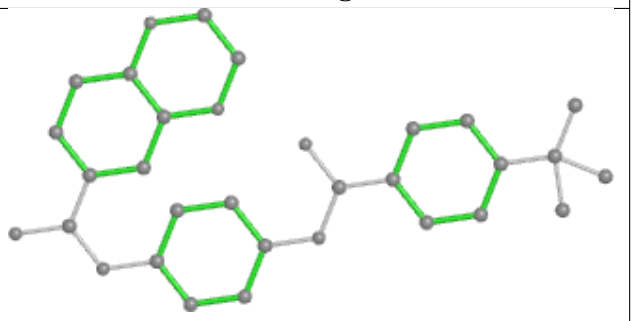
Bond lengths



Bond angles

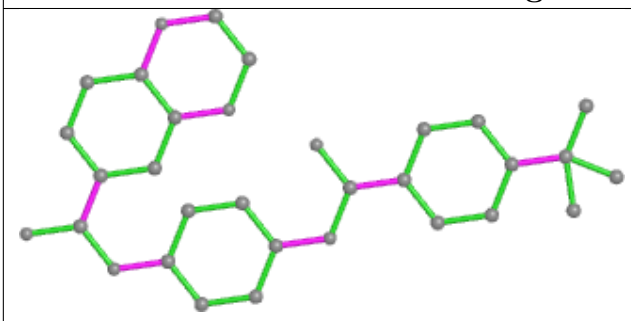


Torsions

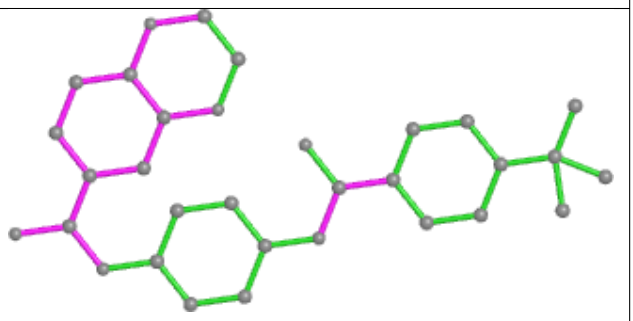


Rings

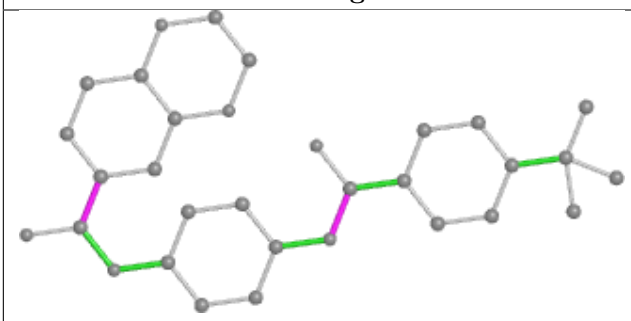
Ligand B7O A 502



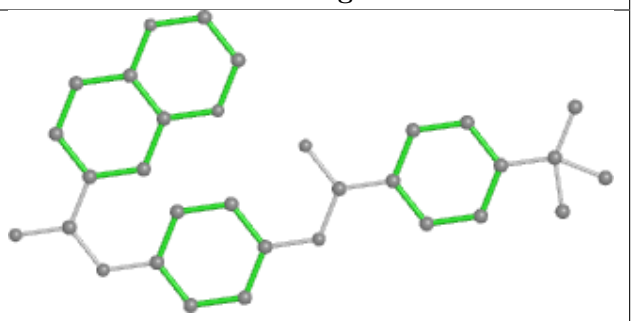
Bond lengths



Bond angles

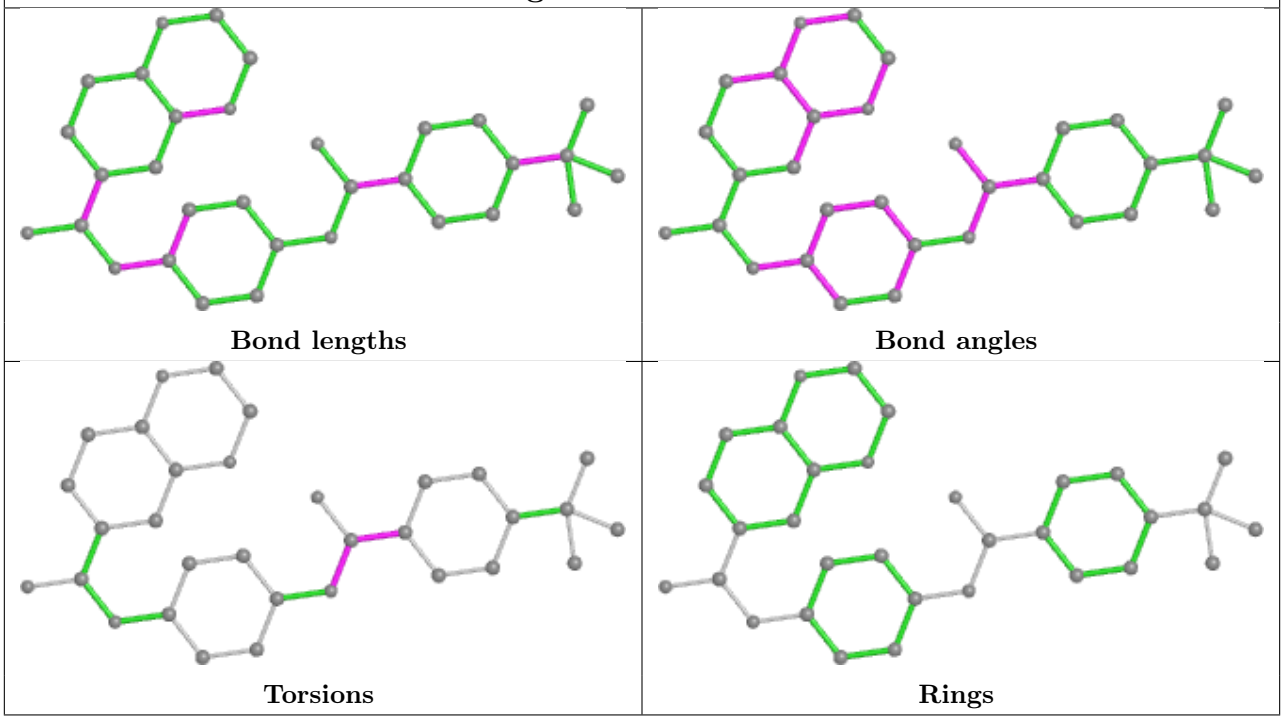


Torsions



Rings

Ligand B7O A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	437/498 (87%)	-0.30	3 (0%) 87 84	26, 44, 84, 112	0
1	B	437/498 (87%)	-0.20	0 100 100	26, 46, 87, 126	0
1	C	442/498 (88%)	0.02	11 (2%) 57 47	30, 61, 103, 119	0
All	All	1316/1494 (88%)	-0.16	14 (1%) 80 75	26, 50, 94, 126	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	111	TYR	4.6
1	C	460	GLY	3.4
1	A	403	SER	3.2
1	A	128	ASP	3.0
1	C	105	ARG	2.9
1	C	127	ASP	2.9
1	C	438	SER	2.5
1	C	76	ASN	2.5
1	C	472	THR	2.3
1	C	469	GLU	2.3
1	C	52	TYR	2.2
1	A	210	GLU	2.0
1	C	108	LEU	2.0
1	C	117	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

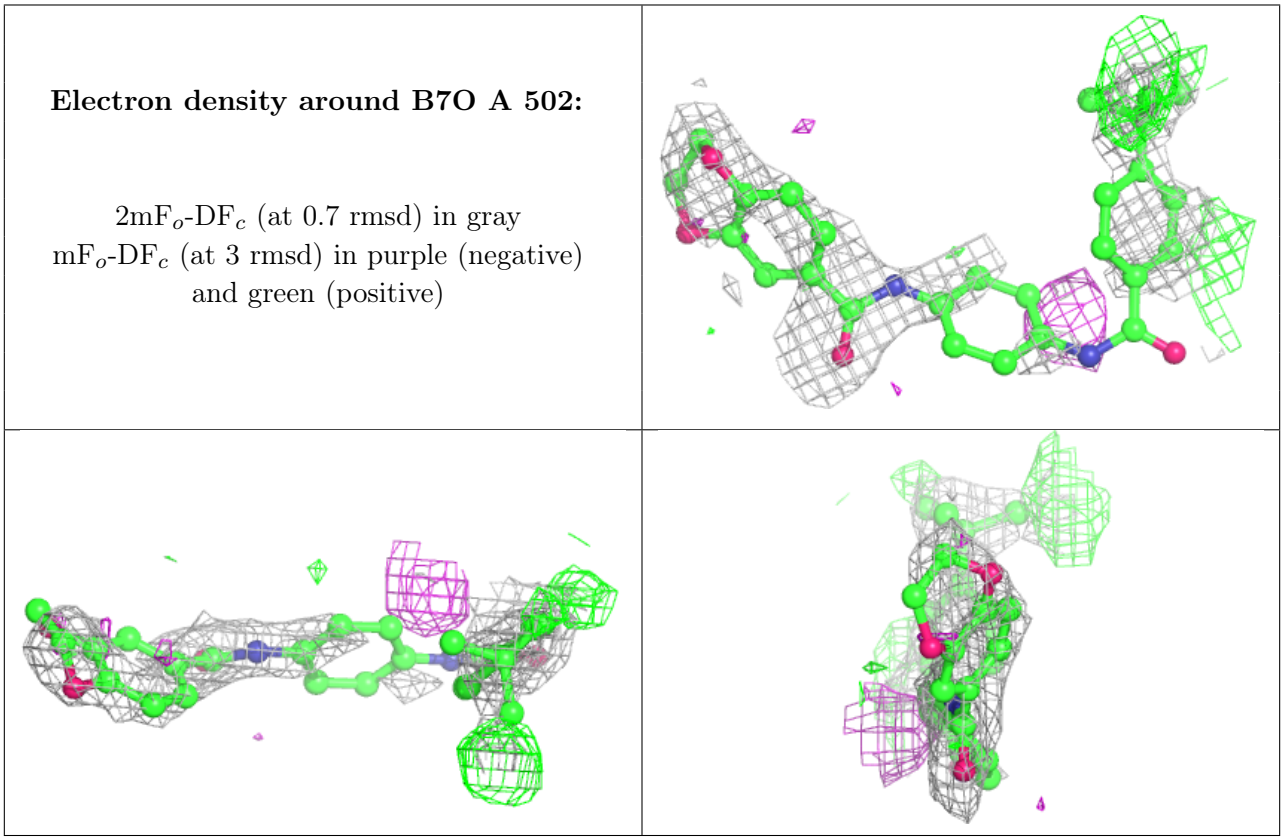
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	B7O	A	502	32/32	0.61	0.46	92,121,134,139	0
2	B7O	C	501	32/32	0.66	0.45	69,113,123,127	0
2	B7O	A	501	32/32	0.74	0.47	65,95,173,176	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.

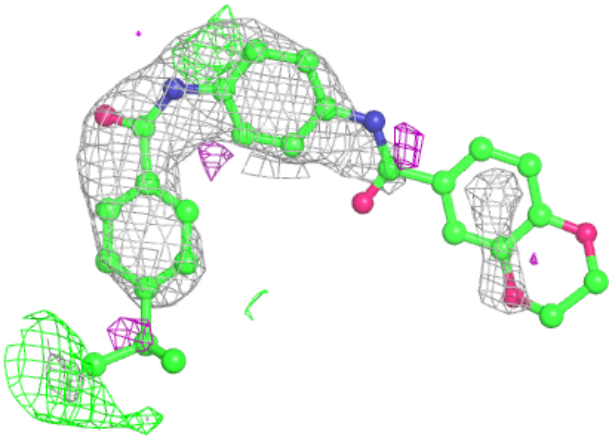
Electron density around B7O A 502:

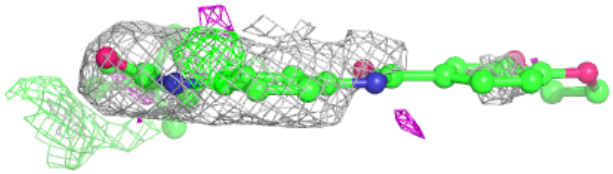
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

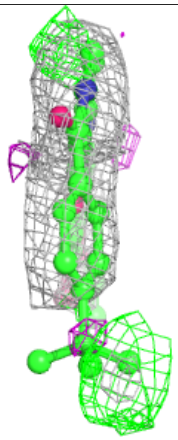


Electron density around B7O C 501:

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

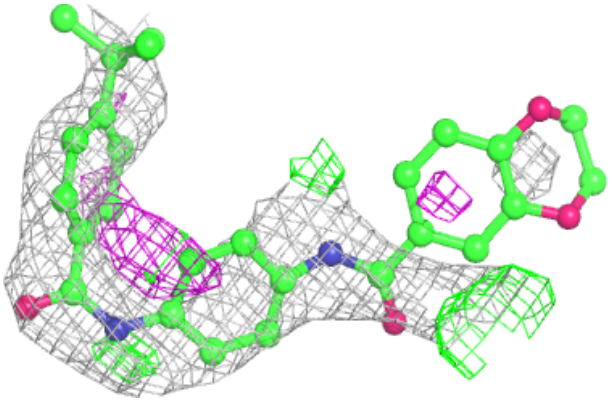


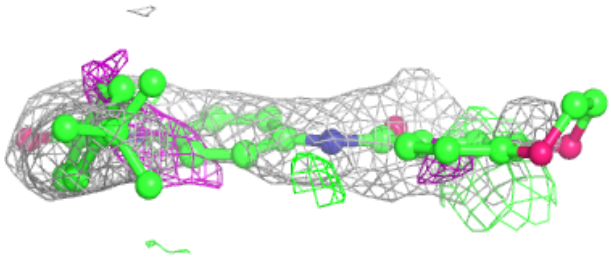


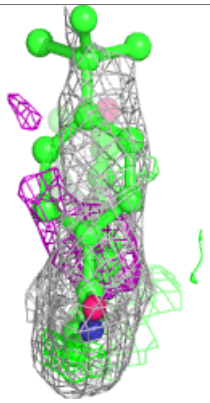


Electron density around B7O A 501:

$2mF_o$-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.