



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:33 PM UTC

PDB ID : 3F3Y / pdb_00003f3y
Title : Crystal structure of human cytosolic sulfotransferase SULT2A1 in complex with PAP and lithocholic acid
Authors : Pan, P.W.; Dong, A.; Amaya, M.; Edwards, A.M.
Deposited on : 2008-10-31
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

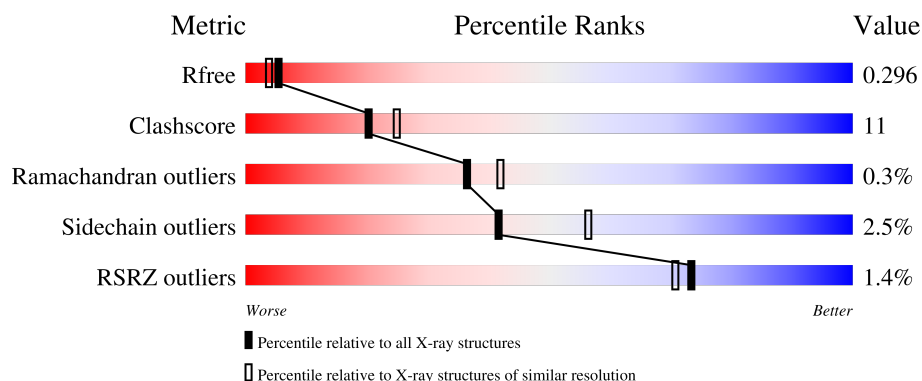
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	
1	B	285	
1	C	285	
1	D	285	

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
3	A3P	C	704	-	-	X	-

2 Entry composition [i](#)

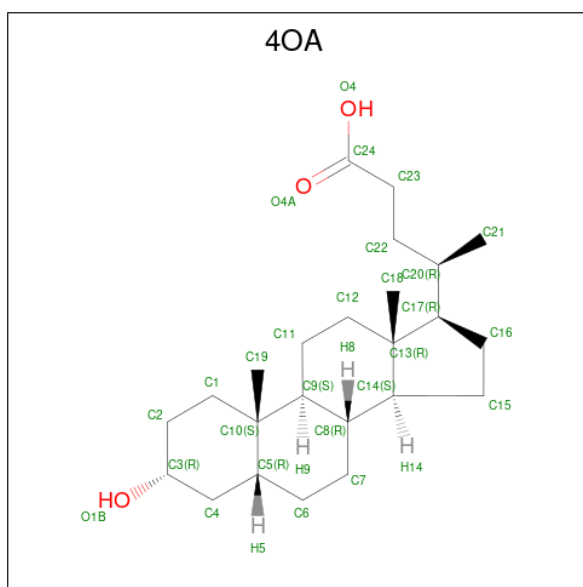
There are 4 unique types of molecules in this entry. The entry contains 9927 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bile salt sulfotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2300	1509	369	410	12			
1	B	282	Total	C	N	O	S	0	0	0
			2297	1507	368	410	12			
1	C	282	Total	C	N	O	S	0	0	0
			2291	1499	370	410	12			
1	D	282	Total	C	N	O	S	0	0	0
			2285	1499	363	411	12			

- Molecule 2 is (3beta,5beta,14beta,17alpha)-3-hydroxycholan-24-oic acid (CCD ID: 4OA) (formula: C₂₄H₄₀O₃).



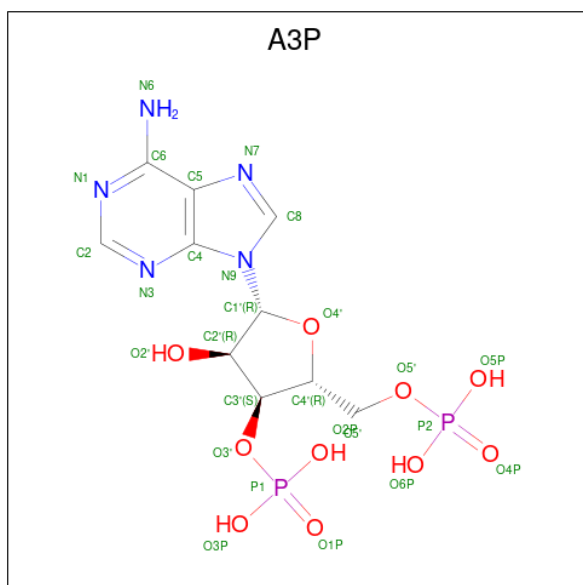
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	24	3		
2	B	1	Total	C	O	0	0
			27	24	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			27	24	3		
2	D	1	Total	C	O	0	0
			27	24	3		

- Molecule 3 is ADENOSINE-3'-5'-DIPHOSPHATE (CCD ID: A3P) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	125	Total	O	0	0
			125	125		
4	C	121	Total	O	0	0
			121	121		

Continued on next page...

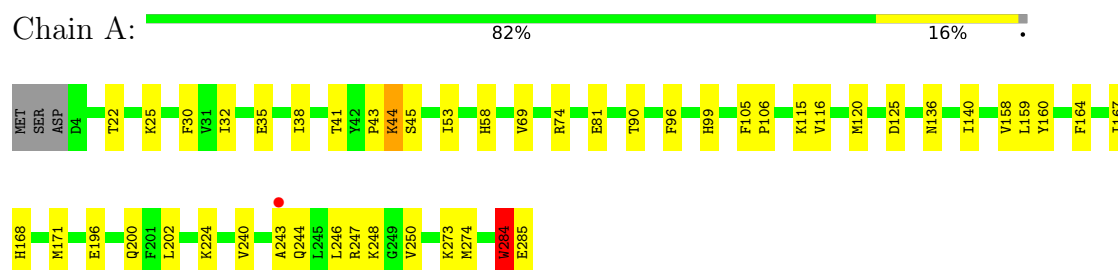
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	137	Total	O	0	0
			137	137		

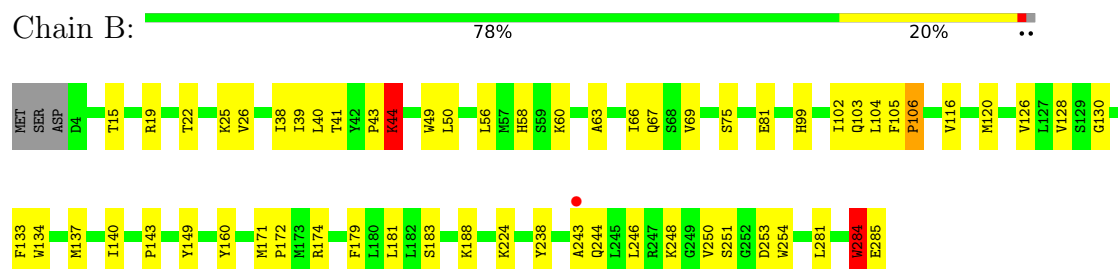
3 Residue-property plots [i](#)

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.

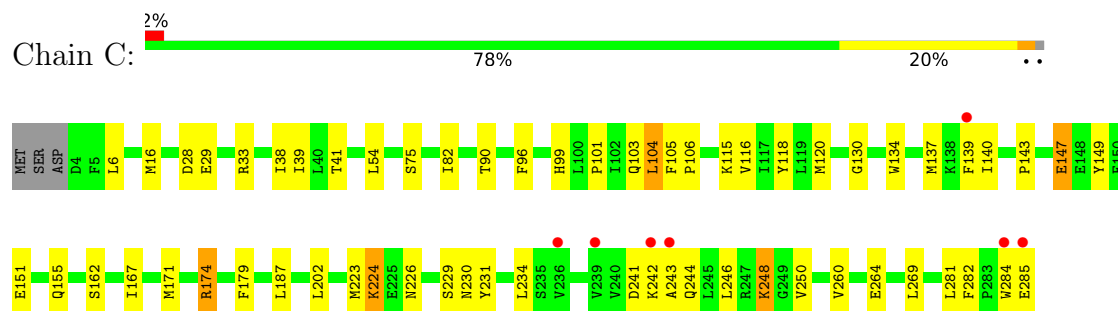
- Molecule 1: Bile salt sulfotransferase



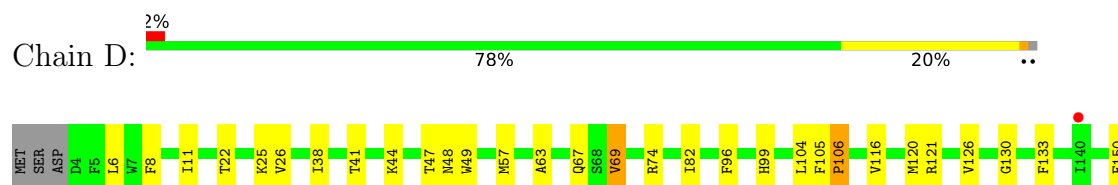
- Molecule 1: Bile salt sulfotransferase

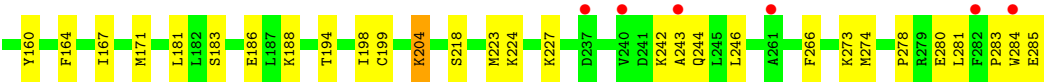


- Molecule 1: Bile salt sulfotransferase



- Molecule 1: Bile salt sulfotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.39Å 96.18Å 159.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.20) 99.0 (30.00-2.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.21 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.299 0.240 , 0.296	Depositor DCC
R_{free} test set	1264 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9927	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2862e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OA, A3P

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	1.13	7/2372 (0.3%)	0.91	1/3215 (0.0%)
1	B	1.07	4/2368 (0.2%)	0.94	3/3210 (0.1%)
1	C	1.04	0/2362	0.88	2/3203 (0.1%)
1	D	1.04	1/2357 (0.0%)	0.94	2/3196 (0.1%)
All	All	1.07	12/9459 (0.1%)	0.92	8/12824 (0.1%)

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	1
1	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	45	SER	N-CA	10.79	1.59	1.46
1	B	44	LYS	CD-CE	8.91	1.79	1.52
1	B	44	LYS	CB-CG	7.53	1.75	1.52
1	B	69	VAL	CA-C	5.99	1.56	1.52
1	A	90	THR	CA-CB	5.53	1.61	1.53
1	D	69	VAL	CA-C	5.53	1.57	1.52
1	A	44	LYS	CA-C	5.28	1.59	1.52
1	B	102	ILE	N-CA	-5.26	1.40	1.46
1	A	74	ARG	C-O	-5.24	1.17	1.24
1	A	53	ILE	CA-CB	-5.19	1.48	1.54
1	A	69	VAL	CA-C	5.18	1.56	1.52
1	A	247	ARG	CZ-NH2	5.05	1.40	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	SER	CA-C-N	6.03	125.99	120.03
1	B	75	SER	C-N-CA	6.03	125.99	120.03
1	C	241	ASP	CB-CA-C	-5.90	109.78	116.63
1	C	187	LEU	N-CA-C	-5.49	105.38	111.36
1	D	133	PHE	N-CA-C	5.37	116.82	111.07
1	B	284	TRP	N-CA-C	-5.33	100.63	108.99
1	D	96	PHE	N-CA-C	5.20	116.19	108.60
1	A	125	ASP	N-CA-C	5.02	116.83	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	TRP	Peptide
1	B	284	TRP	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	2300	0	2198	39	0
1	B	2297	0	2182	58	0
1	C	2291	0	2173	45	0
1	D	2285	0	2151	61	0
2	A	27	0	39	1	0
2	B	27	0	39	3	0
2	C	27	0	39	1	0
2	D	27	0	39	2	0
3	A	27	0	11	1	0
3	B	27	0	11	1	0
3	C	27	0	11	9	0
3	D	27	0	11	4	0
4	A	155	0	0	2	0
4	B	125	0	0	6	0
4	C	121	0	0	5	1
4	D	137	0	0	14	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9927	0	8904	207	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 11.

All (207) 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:44:LYS:CB	1:B:44:LYS:CG	1.75	1.61
1:B:44:LYS:CD	1:B:44:LYS:CE	1.79	1.54
1:D:243:ALA:CB	1:D:244:GLN:HA	1.63	1.26
1:D:266:PHE:HB2	4:D:537:HOH:O	1.28	1.25
1:A:243:ALA:CB	1:A:244:GLN:HA	1.70	1.19
1:B:243:ALA:CB	1:B:244:GLN:HA	1.75	1.13
1:C:223:MET:CE	3:C:704:A3P:HN61	1.62	1.12
1:C:243:ALA:CB	1:C:244:GLN:HA	1.76	1.12
1:A:243:ALA:HB1	1:A:244:GLN:HA	1.22	1.10
1:D:243:ALA:HB1	1:D:244:GLN:HA	1.14	1.10
1:B:243:ALA:HB1	1:B:244:GLN:HA	1.16	1.09
1:D:223:MET:HE3	3:D:703:A3P:HN61	1.14	1.08
1:C:223:MET:HE2	3:C:704:A3P:HN61	0.90	1.06
1:C:243:ALA:HB1	1:C:244:GLN:HA	1.07	1.03
1:D:49:TRP:CD1	1:D:223:MET:HE1	1.96	1.00
1:D:223:MET:HE3	3:D:703:A3P:N6	1.74	1.00
1:C:223:MET:HE2	3:C:704:A3P:N6	1.75	0.99
1:C:223:MET:HE1	3:C:704:A3P:N7	1.76	0.99
1:D:164:PHE:HD2	1:D:274:MET:HE3	1.30	0.96
1:D:243:ALA:HB1	1:D:244:GLN:CA	1.98	0.93
1:D:243:ALA:CB	1:D:244:GLN:CA	2.47	0.93
1:C:243:ALA:HB1	1:C:244:GLN:CA	1.98	0.92
1:D:223:MET:CE	3:D:703:A3P:HN61	1.83	0.90
1:B:243:ALA:HB1	1:B:244:GLN:CA	2.04	0.88
1:A:243:ALA:CB	1:A:244:GLN:CA	2.52	0.87
1:D:164:PHE:CD2	1:D:274:MET:HE3	2.10	0.86
1:A:243:ALA:HB1	1:A:244:GLN:CA	2.04	0.86
1:A:243:ALA:HB3	1:A:244:GLN:HA	1.60	0.84
1:D:243:ALA:HB3	1:D:244:GLN:HA	1.57	0.82
1:C:223:MET:CE	3:C:704:A3P:N7	2.43	0.82
1:D:49:TRP:HD1	1:D:223:MET:HE1	1.44	0.82
1:B:44:LYS:CB	1:B:44:LYS:CD	2.57	0.82
1:C:38:ILE:HB	1:C:116:VAL:HG12	1.62	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:CZ	4:B:535:HOH:O	2.34	0.81
1:C:243:ALA:CB	1:C:244:GLN:CA	2.60	0.79
1:C:28:ASP:CB	4:C:516:HOH:O	2.31	0.78
1:B:133:PHE:CE2	4:B:535:HOH:O	2.36	0.77
1:B:284:TRP:HB2	1:B:285:GLU:CB	2.15	0.76
1:D:150:PHE:HZ	4:D:537:HOH:O	1.71	0.74
1:A:168:HIS:HE1	1:A:274:MET:HE2	1.52	0.74
1:B:44:LYS:CE	1:B:133:PHE:CD2	2.71	0.73
1:B:38:ILE:HB	1:B:116:VAL:HG12	1.70	0.72
1:A:168:HIS:CE1	1:A:274:MET:CE	2.73	0.72
1:B:243:ALA:CB	1:B:244:GLN:CA	2.58	0.71
1:B:44:LYS:CG	1:B:44:LYS:CA	2.67	0.71
1:B:284:TRP:CA	1:B:285:GLU:CB	2.68	0.71
1:C:223:MET:CE	3:C:704:A3P:N6	2.43	0.70
1:B:44:LYS:CD	1:B:44:LYS:NZ	2.54	0.70
1:A:168:HIS:HE1	1:A:274:MET:CE	2.06	0.69
1:D:38:ILE:HB	1:D:116:VAL:HG12	1.74	0.69
1:B:284:TRP:HA	1:B:285:GLU:CB	2.23	0.69
1:D:243:ALA:HB2	4:D:445:HOH:O	1.91	0.68
1:D:223:MET:CE	3:D:703:A3P:N6	2.47	0.68
1:A:168:HIS:CE1	1:A:274:MET:HE1	2.29	0.67
1:B:248:LYS:HB3	1:B:248:LYS:CE	2.24	0.67
1:C:223:MET:HE1	3:C:704:A3P:C5	2.26	0.66
1:D:130:GLY:HA3	4:D:288:HOH:O	1.96	0.65
1:B:243:ALA:HB3	1:B:244:GLN:HA	1.77	0.65
1:B:137:MET:HE2	2:B:327:4OA:H6A	1.79	0.64
1:D:47:THR:HG21	4:D:536:HOH:O	1.97	0.64
1:C:174:ARG:HA	1:C:179:PHE:CD2	2.33	0.64
1:B:44:LYS:CG	1:B:44:LYS:CE	2.71	0.63
1:C:38:ILE:HG12	1:C:96:PHE:CZ	2.34	0.63
1:B:284:TRP:CB	1:B:285:GLU:CB	2.78	0.62
1:B:99:HIS:HB2	1:B:160:TYR:CE2	2.35	0.61
1:D:160:TYR:HB3	4:D:551:HOH:O	2.00	0.61
1:D:8:PHE:HE2	1:D:104:LEU:HD22	1.66	0.60
1:C:224:LYS:HA	1:C:246:LEU:HD13	1.84	0.60
1:A:168:HIS:CE1	1:A:274:MET:HE2	2.33	0.60
1:D:49:TRP:CD1	1:D:223:MET:CE	2.78	0.60
1:C:134:TRP:CE3	1:C:140:ILE:HD13	2.36	0.59
1:A:58:HIS:HD2	4:B:366:HOH:O	1.86	0.59
1:B:44:LYS:CD	1:B:44:LYS:CA	2.81	0.59
1:D:126:VAL:HA	4:D:532:HOH:O	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:GLN:HG2	1:C:104:LEU:HD13	1.84	0.58
1:D:63:ALA:O	1:D:67:GLN:HG3	2.03	0.58
1:B:60:LYS:HE3	4:B:443:HOH:O	2.04	0.58
1:A:164:PHE:HD2	1:A:274:MET:HE3	1.68	0.57
1:B:44:LYS:HB2	1:B:126:VAL:HG13	1.86	0.57
1:B:39:ILE:HG23	1:B:50:LEU:HD23	1.86	0.57
1:D:194:THR:O	1:D:198:ILE:HD12	2.04	0.56
1:D:227:LYS:HG2	4:D:384:HOH:O	2.04	0.56
1:A:273:LYS:O	1:A:274:MET:HE2	2.06	0.56
1:D:183:SER:O	1:D:186:GLU:HG2	2.06	0.56
1:D:224:LYS:HA	1:D:246:LEU:HD13	1.87	0.56
1:D:167:ILE:O	1:D:171:MET:HG2	2.06	0.55
1:D:285:GLU:CG	4:D:291:HOH:O	2.53	0.55
1:B:248:LYS:CE	1:B:253:ASP:HB2	2.36	0.55
1:B:43:PRO:O	1:B:44:LYS:HB2	2.07	0.54
1:A:284:TRP:HB2	1:A:285:GLU:CB	2.38	0.54
1:C:115:LYS:HD2	1:C:202:LEU:HD23	1.90	0.53
1:D:120:MET:HE3	1:D:284:TRP:CH2	2.43	0.53
1:D:284:TRP:HB2	1:D:285:GLU:HA	1.90	0.53
1:C:120:MET:HE2	1:C:167:ILE:HD12	1.91	0.52
1:A:35:GLU:O	4:A:400:HOH:O	2.19	0.52
1:A:196:GLU:O	1:A:200:GLN:HG3	2.09	0.52
1:D:121:ARG:NH1	4:D:532:HOH:O	2.42	0.52
1:C:151:GLU:O	1:C:155:GLN:HG3	2.11	0.51
1:D:99:HIS:HB2	1:D:160:TYR:CE2	2.45	0.51
1:D:218:SER:O	1:D:223:MET:CE	2.58	0.51
1:C:41:THR:O	1:C:99:HIS:HA	2.10	0.51
1:C:143:PRO:HG3	1:C:149:TYR:HB2	1.91	0.51
1:B:41:THR:O	1:B:99:HIS:HA	2.12	0.50
1:C:243:ALA:HB2	4:C:290:HOH:O	2.11	0.50
1:C:130:GLY:O	1:C:134:TRP:CD1	2.64	0.50
1:B:128:VAL:HG21	1:B:254:TRP:HA	1.94	0.50
1:D:243:ALA:HB3	1:D:244:GLN:CA	2.34	0.49
1:B:238:TYR:CE2	2:B:327:4OA:H18	2.47	0.49
1:D:69:VAL:HG12	1:D:74:ARG:HG3	1.93	0.49
1:A:99:HIS:HB2	1:A:160:TYR:CE2	2.47	0.49
1:B:56:LEU:HD21	1:B:66:ILE:HD13	1.95	0.48
1:A:273:LYS:C	1:A:274:MET:HE2	2.38	0.48
1:A:224:LYS:HA	1:A:246:LEU:HD13	1.96	0.48
1:B:44:LYS:HE3	1:B:133:PHE:CD2	2.49	0.48
1:B:171:MET:HE1	1:B:181:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:TYR:OH	1:C:167:ILE:HD13	2.14	0.48
1:A:38:ILE:HB	1:A:116:VAL:HG12	1.95	0.48
1:A:164:PHE:CD2	1:A:274:MET:HE3	2.48	0.48
1:D:285:GLU:HG3	4:D:291:HOH:O	2.13	0.48
1:B:120:MET:O	1:B:183:SER:HA	2.13	0.48
1:B:174:ARG:HA	1:B:179:PHE:CD2	2.48	0.47
2:D:328:4OA:H21A	2:D:328:4OA:H12	1.95	0.47
1:C:223:MET:CE	3:C:704:A3P:C5	2.92	0.47
1:C:134:TRP:HB2	4:C:355:HOH:O	2.15	0.47
1:B:40:LEU:HD11	1:B:116:VAL:HB	1.98	0.46
1:B:130:GLY:O	1:B:134:TRP:CD1	2.68	0.46
1:B:105:PHE:CD1	1:B:106:PRO:HD2	2.49	0.46
1:D:48:ASN:ND2	4:D:385:HOH:O	2.41	0.46
1:B:248:LYS:NZ	3:B:701:A3P:O1P	2.48	0.46
1:D:41:THR:OG1	1:D:99:HIS:CE1	2.69	0.46
1:A:41:THR:O	1:A:99:HIS:HA	2.14	0.46
1:A:44:LYS:NZ	3:A:702:A3P:H5'1	2.30	0.46
1:B:63:ALA:O	1:B:67:GLN:HG3	2.16	0.46
1:B:224:LYS:HA	1:B:246:LEU:HD13	1.97	0.46
2:B:327:4OA:H21A	2:B:327:4OA:H12	1.97	0.46
1:D:120:MET:HE3	1:D:284:TRP:HH2	1.81	0.46
1:A:41:THR:OG1	1:A:99:HIS:CE1	2.69	0.46
1:A:22:THR:OG1	1:A:81:GLU:OE1	2.32	0.46
1:B:44:LYS:CD	1:B:44:LYS:HA	2.45	0.46
1:D:284:TRP:CB	1:D:285:GLU:HA	2.45	0.46
1:B:44:LYS:NZ	1:B:133:PHE:CD2	2.84	0.46
1:D:47:THR:CG2	4:D:536:HOH:O	2.60	0.46
2:A:326:4OA:H12	2:A:326:4OA:H21A	1.99	0.45
1:A:115:LYS:HD2	1:A:202:LEU:HD23	1.98	0.45
1:D:49:TRP:HD1	1:D:223:MET:CE	2.20	0.45
1:C:226:ASN:HB3	1:C:229:SER:HB2	1.99	0.45
1:B:137:MET:SD	4:B:535:HOH:O	2.60	0.45
1:D:273:LYS:C	1:D:274:MET:HE2	2.41	0.45
1:A:22:THR:HA	1:A:25:LYS:HE2	1.98	0.45
1:C:248:LYS:NZ	1:C:248:LYS:HB2	2.32	0.45
1:A:248:LYS:HB2	1:A:248:LYS:HE2	1.66	0.45
1:C:33:ARG:NH1	1:C:90:THR:O	2.45	0.44
1:D:105:PHE:O	1:D:106:PRO:C	2.59	0.44
1:A:136:ASN:HB3	1:A:240:VAL:O	2.17	0.44
1:D:105:PHE:CD1	1:D:106:PRO:HD2	2.53	0.44
1:B:120:MET:HE1	1:B:281:LEU:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:VAL:O	1:C:264:GLU:HG3	2.17	0.44
1:B:22:THR:O	1:B:26:VAL:HG23	2.18	0.43
1:C:29:GLU:HG3	4:C:541:HOH:O	2.17	0.43
1:C:105:PHE:O	1:C:106:PRO:C	2.61	0.43
1:A:105:PHE:O	1:A:106:PRO:C	2.61	0.43
1:D:25:LYS:O	1:D:26:VAL:C	2.61	0.43
1:A:38:ILE:HG12	1:A:96:PHE:CZ	2.53	0.43
1:A:167:ILE:O	1:A:171:MET:HG2	2.18	0.43
1:D:8:PHE:CE2	1:D:104:LEU:HD22	2.50	0.43
2:D:328:4OA:H21	4:D:312:HOH:O	2.18	0.43
1:D:44:LYS:HG3	1:D:130:GLY:HA2	2.00	0.43
1:B:143:PRO:HG3	1:B:149:TYR:HB2	2.00	0.42
1:B:43:PRO:O	1:B:44:LYS:CB	2.67	0.42
1:B:251:SER:HB3	4:B:290:HOH:O	2.19	0.42
1:C:39:ILE:HD11	1:C:54:LEU:HD12	2.00	0.42
1:D:22:THR:O	1:D:26:VAL:HG23	2.19	0.42
1:D:57:MET:HE1	1:D:198:ILE:HG22	2.01	0.42
1:A:43:PRO:O	1:A:44:LYS:HB2	2.20	0.42
1:D:281:LEU:O	1:D:283:PRO:HD3	2.20	0.42
1:B:171:MET:N	1:B:172:PRO:CD	2.83	0.42
1:C:284:TRP:HA	1:C:285:GLU:HA	1.73	0.42
1:D:218:SER:O	1:D:223:MET:HE2	2.19	0.42
1:B:22:THR:HA	1:B:25:LYS:HE2	2.02	0.42
1:D:218:SER:O	1:D:223:MET:HE3	2.20	0.42
1:A:41:THR:HG1	1:A:99:HIS:CE1	2.38	0.42
1:C:120:MET:HE1	1:C:282:PHE:HE1	1.85	0.42
1:C:16:MET:HE3	1:C:139:PHE:HA	2.02	0.41
1:C:171:MET:O	1:C:174:ARG:HB3	2.19	0.41
1:A:105:PHE:CD1	1:A:106:PRO:HD2	2.55	0.41
1:A:243:ALA:HB3	1:A:244:GLN:CA	2.37	0.41
1:B:19:ARG:HD3	1:B:81:GLU:OE2	2.21	0.41
1:B:49:TRP:HH2	1:B:188:LYS:HA	1.86	0.41
1:C:137:MET:HE2	2:C:329:4OA:H6A	2.01	0.41
1:D:243:ALA:HB3	1:D:244:GLN:NE2	2.35	0.41
1:A:158:VAL:O	1:A:159:LEU:C	2.64	0.41
1:C:243:ALA:CA	4:C:290:HOH:O	2.68	0.41
1:D:278:PRO:C	1:D:280:GLU:H	2.29	0.41
1:B:105:PHE:O	1:B:106:PRO:C	2.63	0.41
1:D:49:TRP:HH2	1:D:188:LYS:HA	1.86	0.41
1:D:171:MET:HE1	1:D:181:LEU:HD13	2.03	0.41
1:D:199:CYS:HB3	1:D:204:LYS:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ASN:O	1:C:231:TYR:HB2	2.20	0.40
1:C:147:GLU:CD	1:C:147:GLU:H	2.29	0.40
4:A:401:HOH:O	1:B:58:HIS:HD2	2.03	0.40
1:C:101:PRO:HG2	1:C:104:LEU:HD22	2.03	0.40
1:D:11:ILE:HG13	1:D:104:LEU:HD11	2.02	0.40
1:A:30:PHE:HE2	1:A:32:ILE:HD13	1.85	0.40
1:B:44:LYS:NZ	1:B:133:PHE:CE2	2.89	0.40
1:A:248:LYS:HG2	1:A:250:VAL:HG22	2.02	0.40
1:B:103:GLN:HG2	1:B:104:LEU:HD23	2.03	0.40
1:C:223:MET:HE3	3:C:704:A3P:N7	2.32	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)
4:C:311:HOH:O	4:D:565:HOH:O[1_455]	2.19	0.01

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	280/285 (98%)	267 (95%)	12 (4%)	1 (0%)	30	34
1	B	280/285 (98%)	269 (96%)	10 (4%)	1 (0%)	30	34
1	C	280/285 (98%)	268 (96%)	12 (4%)	0	100	100
1	D	280/285 (98%)	267 (95%)	12 (4%)	1 (0%)	30	34
All	All	1120/1140 (98%)	1071 (96%)	46 (4%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	TRP
1	B	44	LYS
1	D	106	PRO

5.3.2 Protein sidechains ⓘ

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	243/263 (92%)	241 (99%)	2 (1%)	73	85
1	B	241/263 (92%)	237 (98%)	4 (2%)	53	69
1	C	240/263 (91%)	226 (94%)	14 (6%)	18	22
1	D	237/263 (90%)	233 (98%)	4 (2%)	53	69
All	All	961/1052 (91%)	937 (98%)	24 (2%)	42	56

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	MET
1	A	140	ILE
1	B	15	THR
1	B	106	PRO
1	B	140	ILE
1	B	250	VAL
1	C	6	LEU
1	C	75	SER
1	C	82	ILE
1	C	104	LEU
1	C	147	GLU
1	C	162	SER
1	C	174	ARG
1	C	224	LYS
1	C	234	LEU
1	C	242	LYS
1	C	248	LYS
1	C	250	VAL
1	C	269	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	281	LEU
1	D	6	LEU
1	D	82	ILE
1	D	204	LYS
1	D	242	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	67	GLN
1	A	200	GLN
1	B	48	ASN
1	B	189	GLN
1	C	48	ASN
1	D	48	ASN
1	D	189	GLN

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](#)

8 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	4OA	D	328	-	30,30,30	0.62	0	47,47,47	0.90	1 (2%)
2	4OA	C	329	-	30,30,30	0.74	0	47,47,47	1.11	3 (6%)
3	A3P	C	704	-	29,29,29	1.35	4 (13%)	44,45,45	1.90	12 (27%)
3	A3P	D	703	-	29,29,29	1.46	4 (13%)	44,45,45	1.97	12 (27%)
2	4OA	A	326	-	30,30,30	0.75	0	47,47,47	0.90	2 (4%)
3	A3P	A	702	-	29,29,29	1.35	3 (10%)	44,45,45	1.93	13 (29%)
3	A3P	B	701	-	29,29,29	1.43	6 (20%)	44,45,45	2.05	13 (29%)
2	4OA	B	327	-	30,30,30	0.64	0	47,47,47	1.00	3 (6%)

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	4OA	D	328	-	-	0/9/67/67	0/4/4/4
2	4OA	C	329	-	-	0/9/67/67	0/4/4/4
3	A3P	C	704	-	-	2/15/31/31	0/3/3/3
3	A3P	D	703	-	-	3/15/31/31	0/3/3/3
2	4OA	A	326	-	-	0/9/67/67	0/4/4/4
3	A3P	A	702	-	-	0/15/31/31	0/3/3/3
3	A3P	B	701	-	-	0/15/31/31	0/3/3/3
2	4OA	B	327	-	-	0/9/67/67	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	A3P	C5-C4	3.88	1.46	1.39
3	D	703	A3P	C5-C4	3.77	1.45	1.39
3	A	702	A3P	C5-C4	3.71	1.45	1.39
3	B	701	A3P	C5-C4	3.60	1.45	1.39
3	A	702	A3P	C5-N7	-3.06	1.33	1.39
3	D	703	A3P	C5-N7	-3.05	1.33	1.39
3	C	704	A3P	P1-O3'	2.94	1.64	1.59
3	B	701	A3P	C5-C6	2.83	1.48	1.41
3	D	703	A3P	C5-C6	2.80	1.48	1.41
3	C	704	A3P	C8-N7	2.78	1.37	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	A3P	C8-N7	2.77	1.37	1.31
3	A	702	A3P	C8-N7	2.75	1.37	1.31
3	B	701	A3P	C4-N9	-2.55	1.32	1.37
3	B	701	A3P	C5-N7	-2.54	1.34	1.39
3	B	701	A3P	C8-N7	2.27	1.36	1.31
3	C	704	A3P	C5-C6	2.26	1.47	1.41
3	B	701	A3P	P1-O3P	-2.24	1.46	1.54

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	703	A3P	C5-C4-N3	-6.29	118.06	126.72
3	A	702	A3P	C5-C4-N3	-5.06	119.75	126.72
3	B	701	A3P	C5-C4-N3	-5.02	119.80	126.72
3	C	704	A3P	C5-C4-N3	-4.90	119.97	126.72
3	C	704	A3P	N3-C2-N1	-4.66	121.53	128.58
3	B	701	A3P	C2-N3-C4	4.65	123.18	111.83
3	D	703	A3P	N3-C4-N9	4.53	134.87	127.17
3	B	701	A3P	N3-C2-N1	-4.39	121.94	128.58
3	A	702	A3P	N3-C2-N1	-4.33	122.02	128.58
3	A	702	A3P	N3-C4-N9	4.08	134.10	127.17
3	D	703	A3P	C2-N3-C4	3.99	121.57	111.83
3	C	704	A3P	C2-N3-C4	3.93	121.43	111.83
3	C	704	A3P	N3-C4-N9	3.91	133.82	127.17
3	A	702	A3P	O4'-C1'-N9	3.84	115.46	108.09
3	D	703	A3P	C4-C5-N7	-3.77	106.28	110.58
3	A	702	A3P	C2-N3-C4	3.74	120.97	111.83
3	B	701	A3P	N3-C4-N9	3.72	133.49	127.17
3	B	701	A3P	O5P-P2-O5'	-3.67	97.10	106.67
3	B	701	A3P	O4'-C1'-N9	3.65	115.10	108.09
3	C	704	A3P	C4-N9-C8	3.52	109.43	105.74
3	D	703	A3P	N3-C2-N1	-3.38	123.47	128.58
3	D	703	A3P	C5-N7-C8	3.14	108.39	103.45
3	B	701	A3P	O3'-P1-O1P	-2.97	98.74	109.33
2	A	326	4OA	C4-C3-C2	-2.96	107.01	110.62
3	B	701	A3P	C4-C5-N7	-2.93	107.24	110.58
3	C	704	A3P	N9-C8-N7	-2.84	109.90	113.94
2	C	329	4OA	O1B-C3-C4	-2.84	104.19	109.84
3	D	703	A3P	O4'-C1'-N9	2.78	113.44	108.09
3	B	701	A3P	C4-N9-C8	2.67	108.54	105.74
3	B	701	A3P	C6-C5-N7	2.66	137.21	132.09
3	C	704	A3P	C4-C5-N7	-2.60	107.61	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	704	A3P	C2-N1-C6	2.60	123.00	118.73
3	C	704	A3P	O4'-C1'-N9	2.55	112.99	108.09
3	B	701	A3P	N9-C8-N7	-2.54	110.33	113.94
2	B	327	4OA	C4-C3-C2	-2.54	107.52	110.62
3	A	702	A3P	N9-C8-N7	-2.51	110.38	113.94
3	D	703	A3P	N9-C8-N7	-2.48	110.42	113.94
3	C	704	A3P	C6-C5-N7	2.47	136.84	132.09
2	C	329	4OA	C11-C9-C8	2.46	115.22	111.78
3	A	702	A3P	C2-N1-C6	2.45	122.76	118.73
3	A	702	A3P	O6P-P2-O5P	2.41	116.86	107.80
3	A	702	A3P	O4'-C1'-C2'	-2.40	101.47	106.62
3	B	701	A3P	C5-N7-C8	2.38	107.19	103.45
3	A	702	A3P	C4-N9-C8	2.37	108.22	105.74
3	C	704	A3P	O2'-C2'-C3'	2.34	117.72	111.19
3	D	703	A3P	C6-C5-N7	2.22	136.37	132.09
3	B	701	A3P	O3P-P1-O2P	2.21	116.10	107.80
3	C	704	A3P	C5-N7-C8	2.15	106.83	103.45
3	A	702	A3P	C5-N7-C8	2.13	106.79	103.45
2	C	329	4OA	C4-C5-C10	-2.10	110.42	112.66
2	A	326	4OA	C5-C4-C3	-2.09	109.56	112.71
3	A	702	A3P	O3P-P1-O2P	2.08	115.61	107.80
3	D	703	A3P	O6P-P2-O5P	2.08	115.61	107.80
2	B	327	4OA	C7-C8-C9	-2.08	108.03	110.52
2	B	327	4OA	C19-C10-C9	-2.05	108.43	111.18
3	A	702	A3P	N6-C6-N1	2.04	122.92	118.38
3	D	703	A3P	O3P-P1-O2P	2.02	115.38	107.80
3	D	703	A3P	C4-N9-C8	2.02	107.86	105.74
2	D	328	4OA	C4-C5-C10	2.00	114.79	112.66

There are no chirality outliers.

All (5) torsion outliers are listed below:

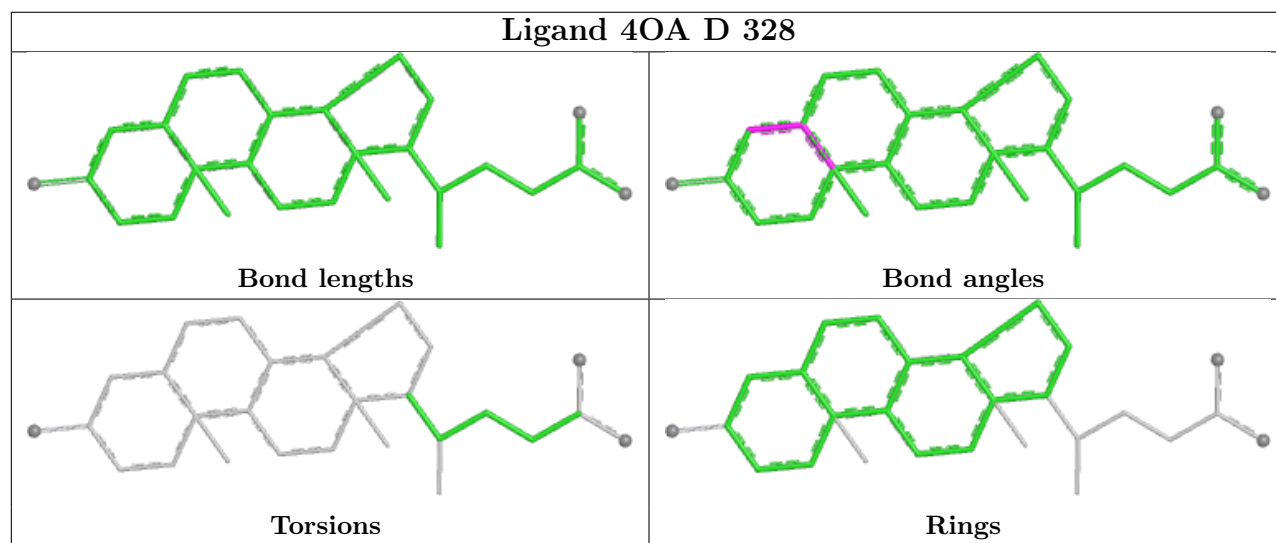
Mol	Chain	Res	Type	Atoms
3	C	704	A3P	C3'-C4'-C5'-O5'
3	D	703	A3P	C5'-O5'-P2-O5P
3	D	703	A3P	C5'-O5'-P2-O4P
3	D	703	A3P	C5'-O5'-P2-O6P
3	C	704	A3P	O4'-C4'-C5'-O5'

There are no ring outliers.

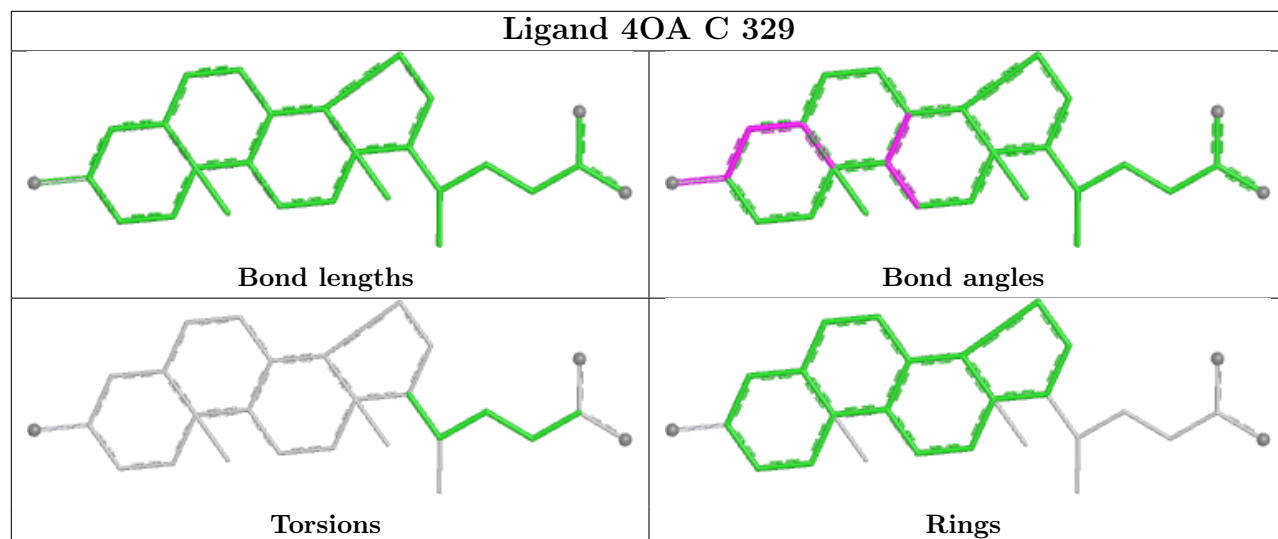
8 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	328	4OA	2	0
2	C	329	4OA	1	0
3	C	704	A3P	9	0
3	D	703	A3P	4	0
2	A	326	4OA	1	0
3	A	702	A3P	1	0
3	B	701	A3P	1	0
2	B	327	4OA	3	0

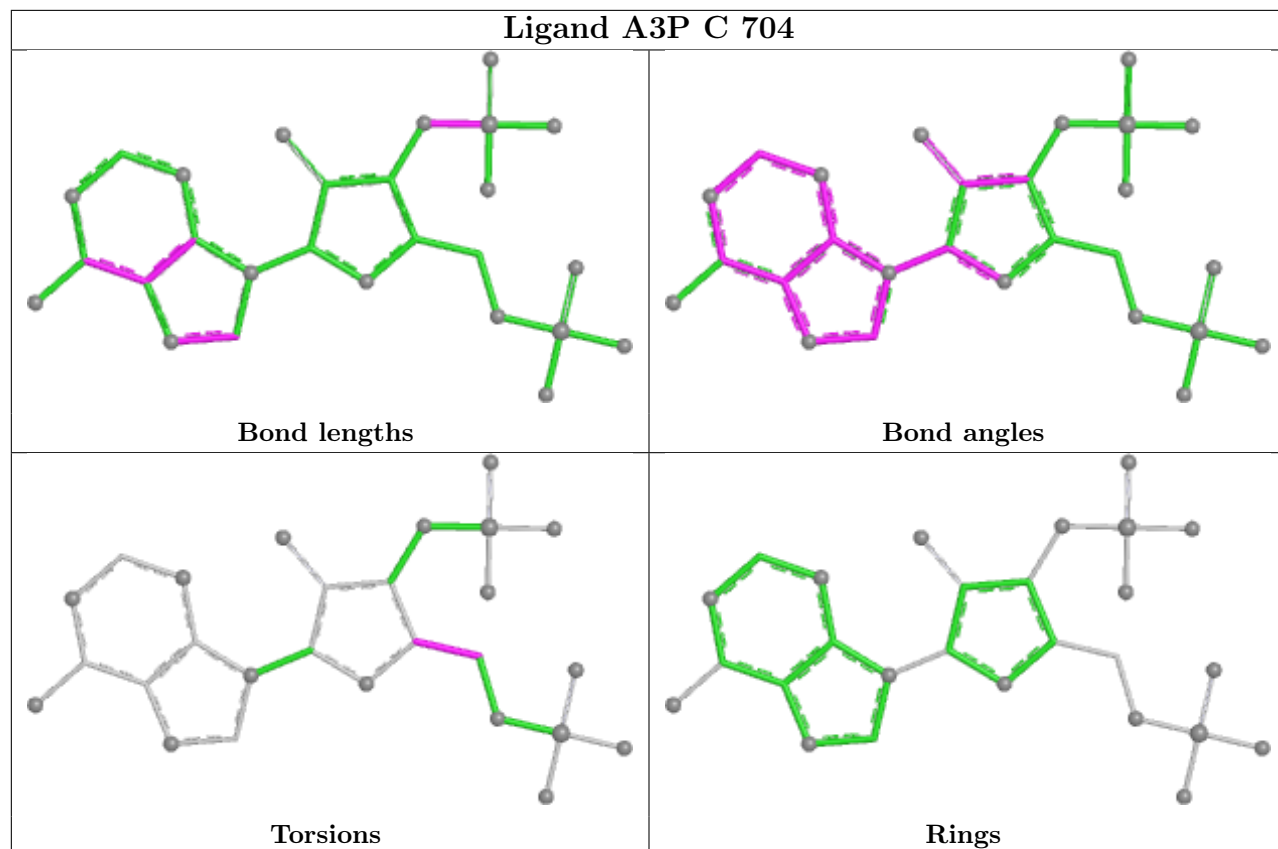
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



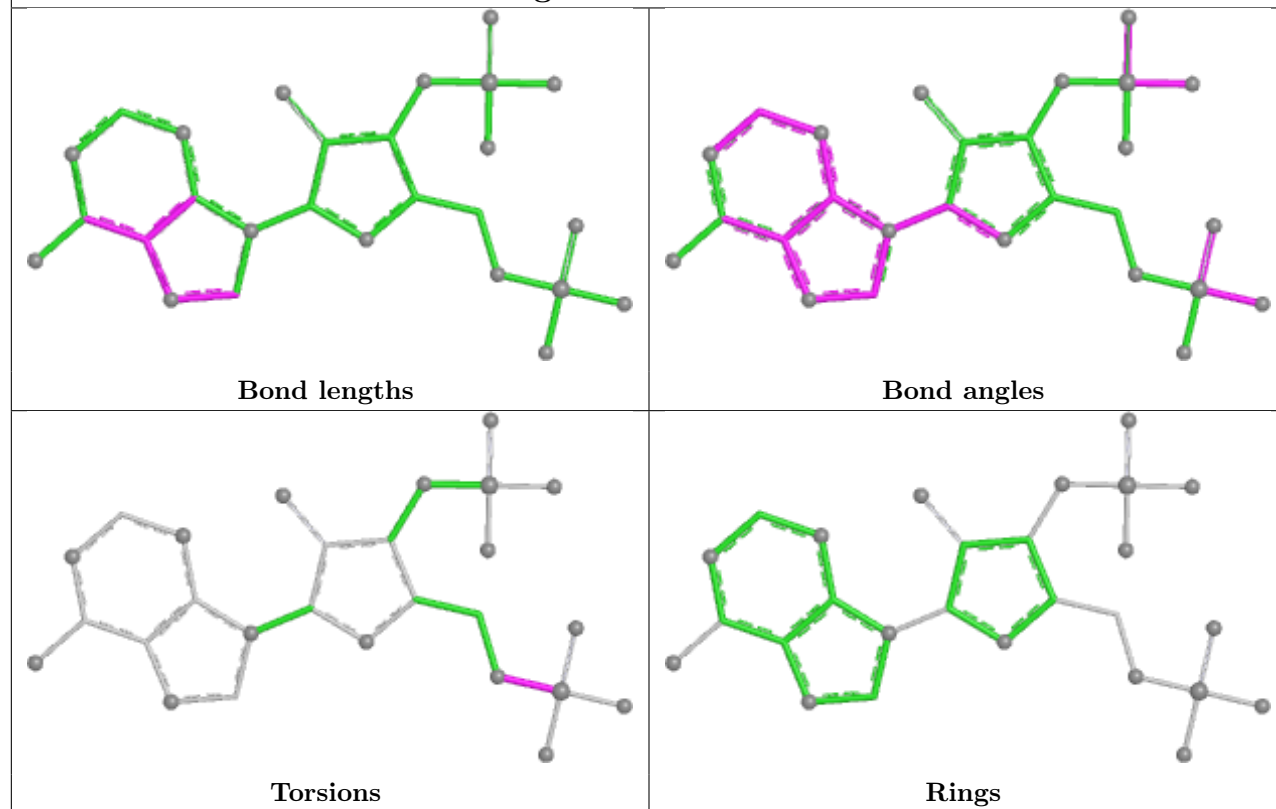
Ligand 4OA C 329



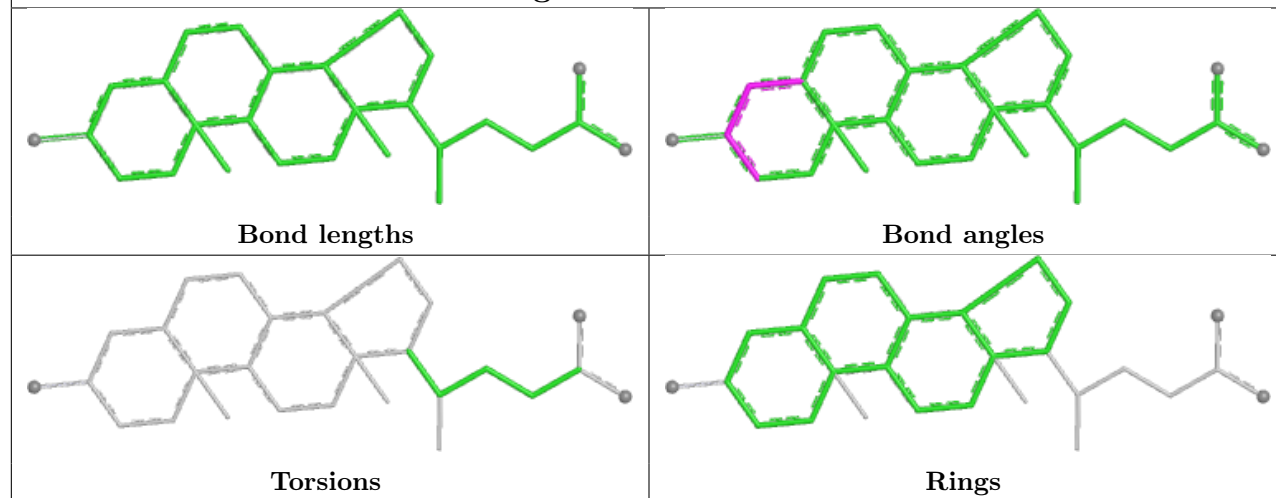
Ligand A3P C 704



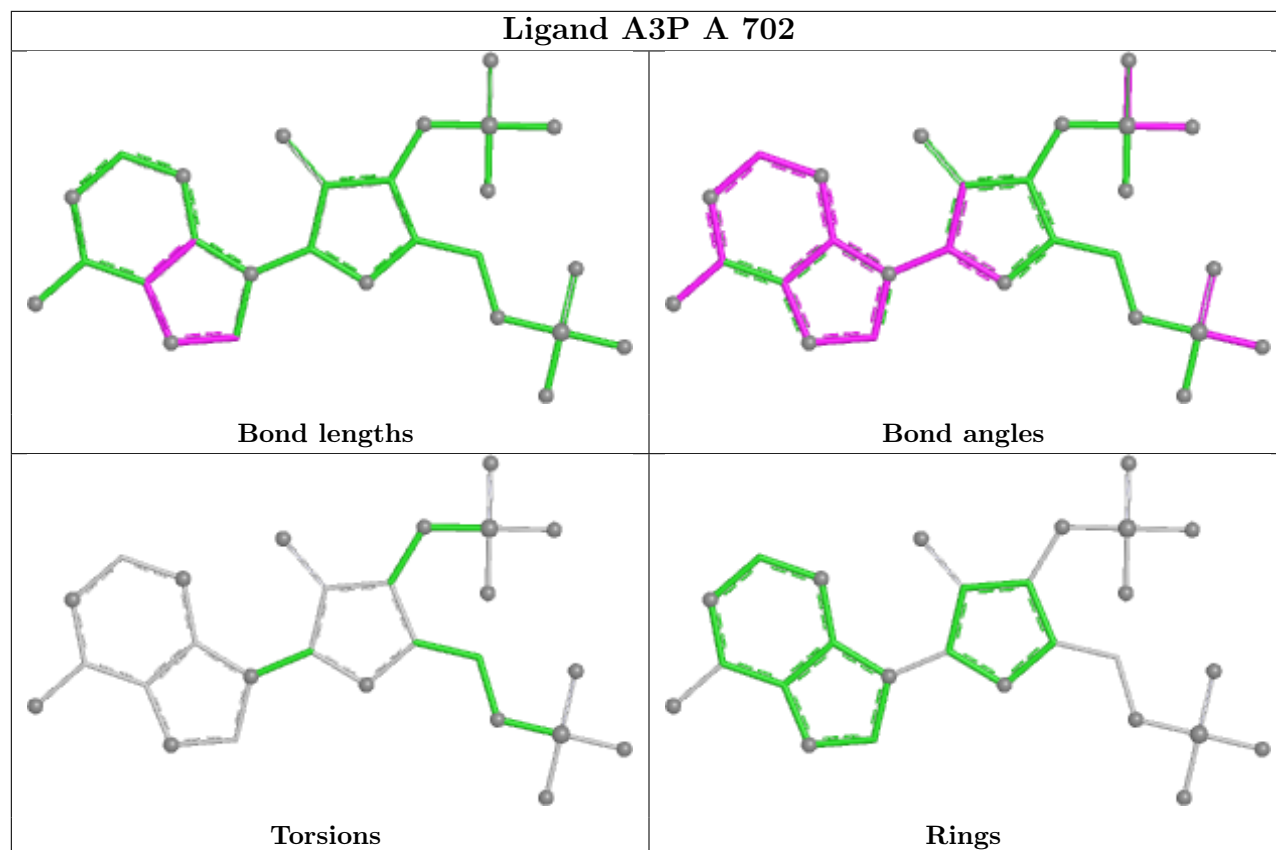
Ligand A3P D 703



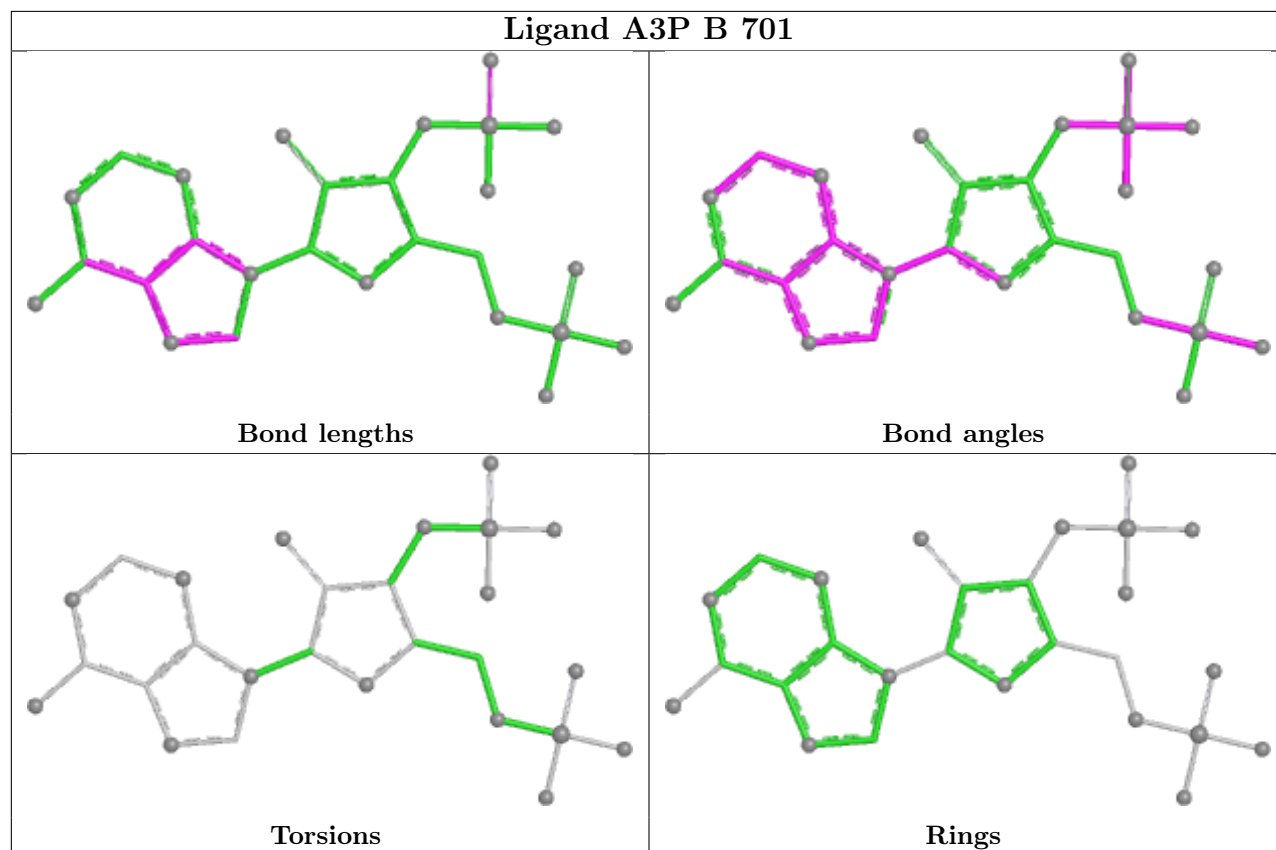
Ligand 4OA A 326

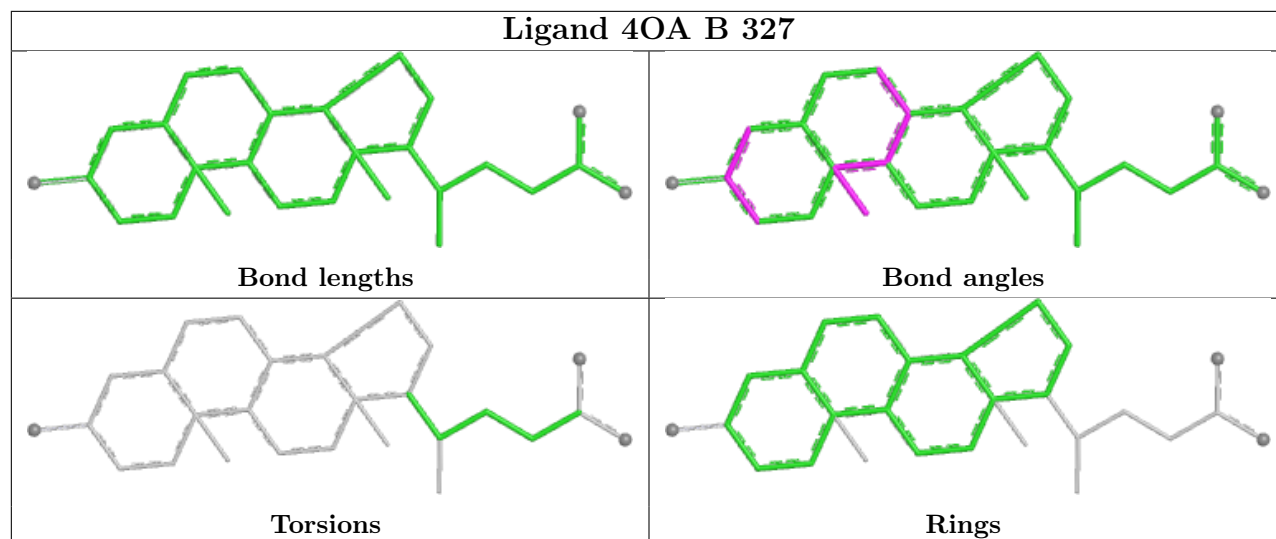


Ligand A3P A 702



Ligand A3P B 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	282/285 (98%)	-0.32	1 (0%) 88 87	5, 26, 45, 56	0
1	B	282/285 (98%)	-0.29	1 (0%) 88 87	5, 27, 47, 61	0
1	C	282/285 (98%)	0.36	7 (2%) 58 55	23, 38, 57, 67	0
1	D	282/285 (98%)	0.32	7 (2%) 58 55	19, 37, 59, 74	0
All	All	1128/1140 (98%)	0.02	16 (1%) 73 71	5, 33, 55, 74	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	243	ALA	4.0
1	B	243	ALA	2.8
1	D	237	ASP	2.5
1	A	243	ALA	2.4
1	C	242	LYS	2.4
1	C	236	VAL	2.4
1	D	140	ILE	2.3
1	D	282	PHE	2.3
1	D	240	VAL	2.2
1	D	261	ALA	2.2
1	C	139	PHE	2.2
1	C	243	ALA	2.1
1	C	284	TRP	2.1
1	C	239	VAL	2.1
1	D	284	TRP	2.1
1	C	285	GLU	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](#)

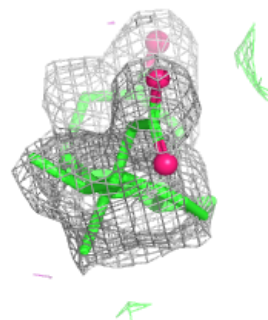
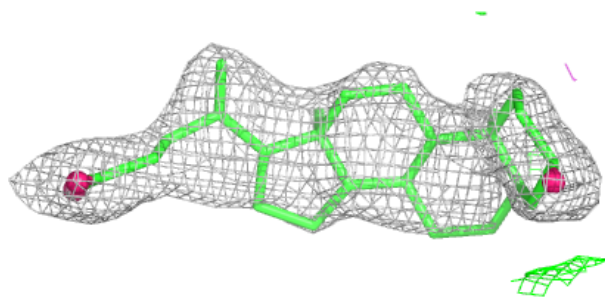
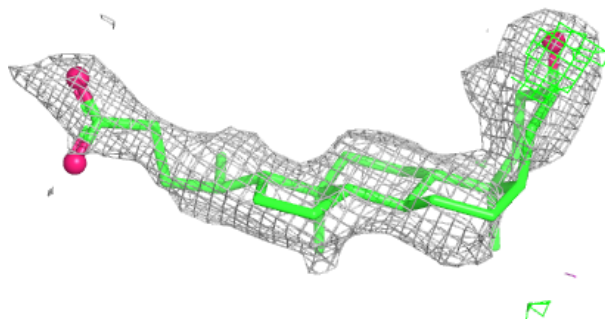
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	4OA	D	328	27/27	0.72	0.17	60,66,67,69	0
2	4OA	C	329	27/27	0.77	0.12	40,46,55,57	0
2	4OA	B	327	27/27	0.80	0.12	42,45,48,49	0
2	4OA	A	326	27/27	0.89	0.09	34,38,46,47	0
3	A3P	C	704	27/27	0.93	0.09	26,31,33,35	0
3	A3P	D	703	27/27	0.95	0.07	24,29,32,32	0
3	A3P	A	702	27/27	0.98	0.05	12,17,21,22	0
3	A3P	B	701	27/27	0.98	0.05	14,20,23,23	0

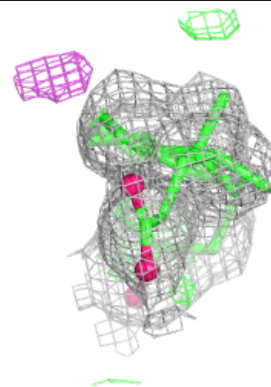
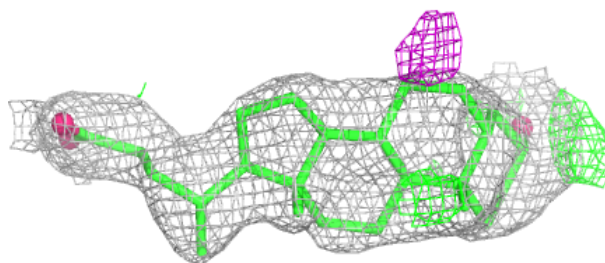
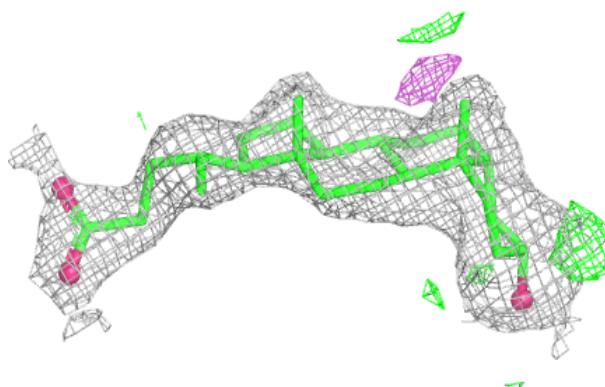
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4OA D 328:

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

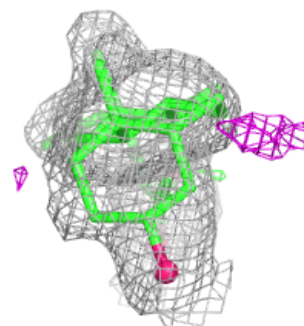
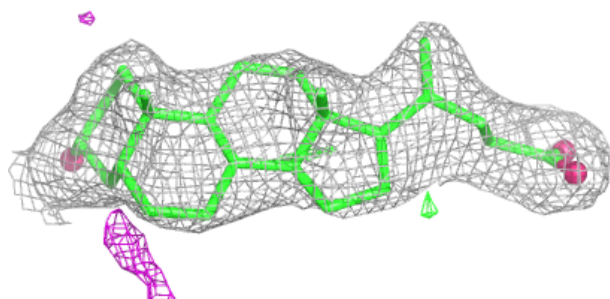
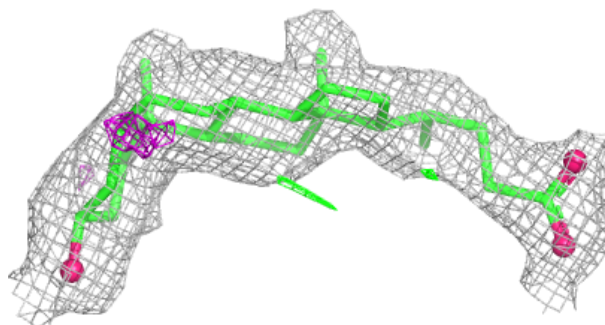
**Electron density around 4OA C 329:**

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

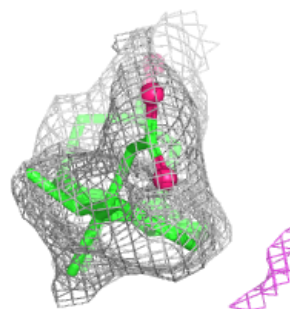
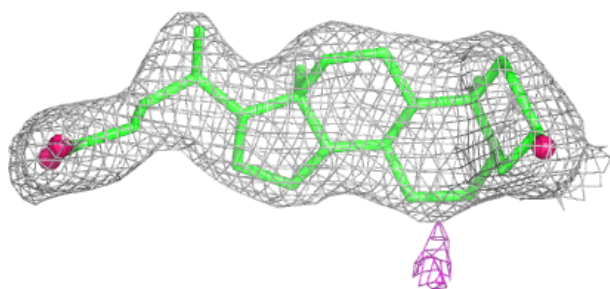
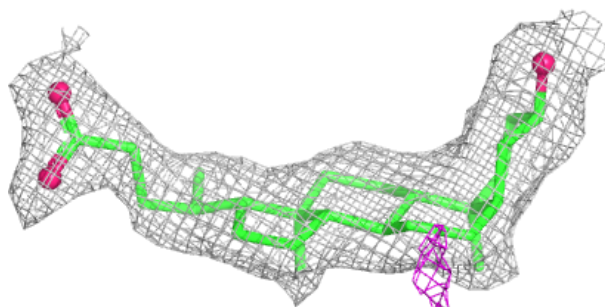


Electron density around 4OA B 327:

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

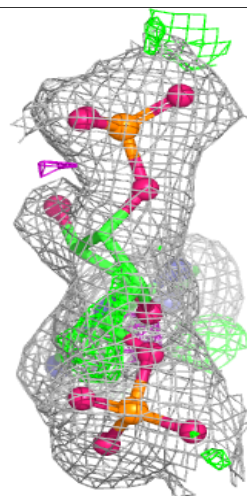
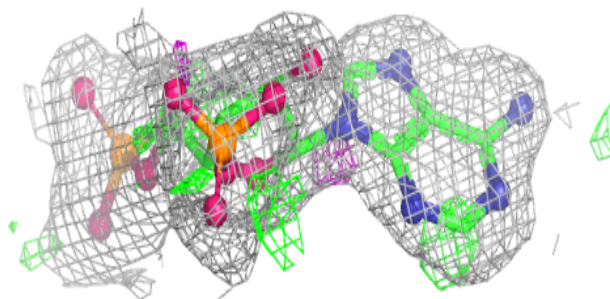
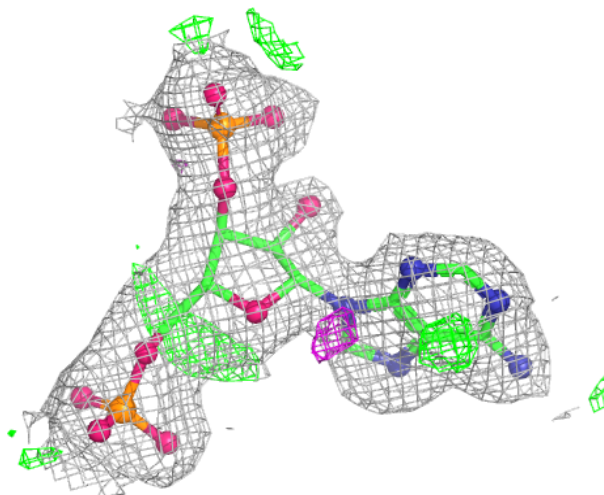
**Electron density around 4OA A 326:**

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



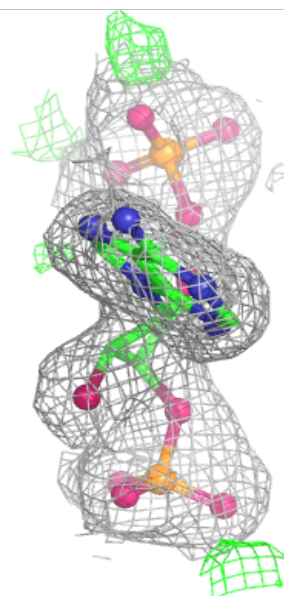
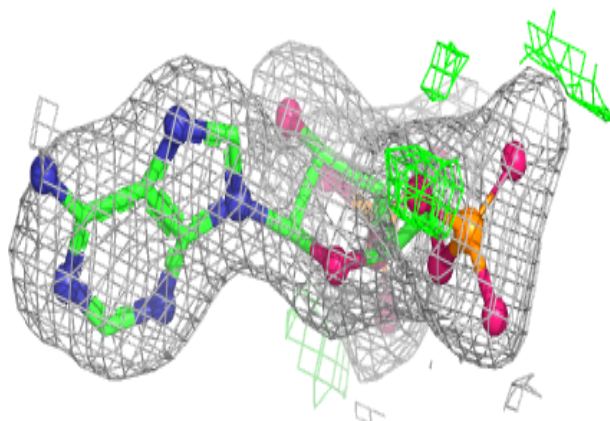
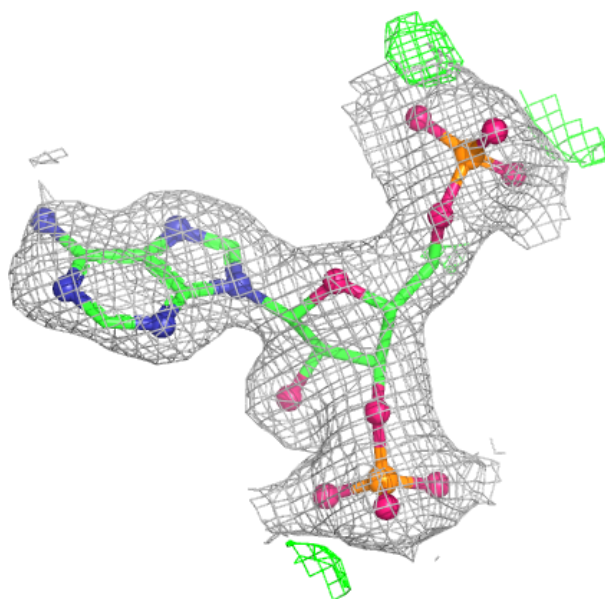
Electron density around A3P C 704:

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



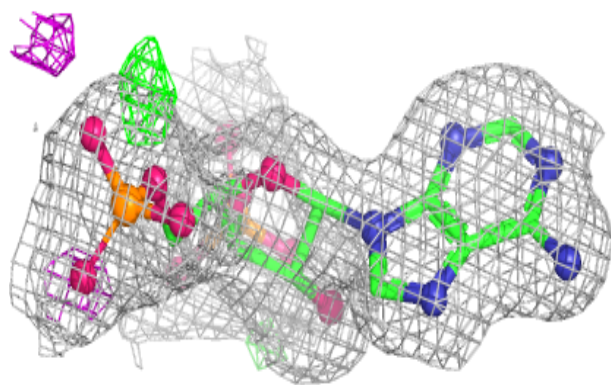
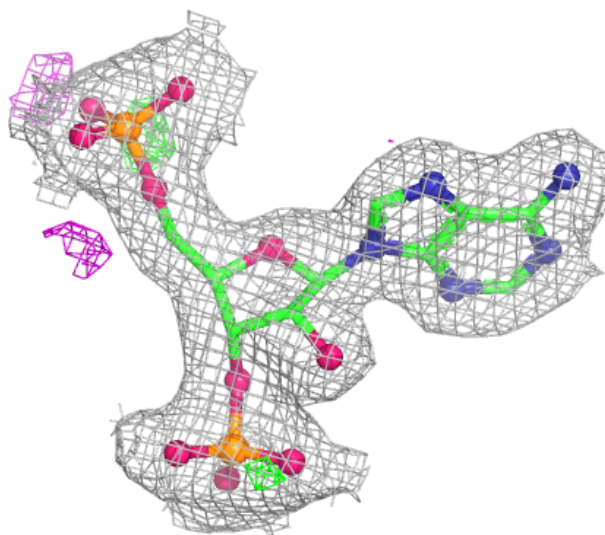
Electron density around A3P D 703:

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



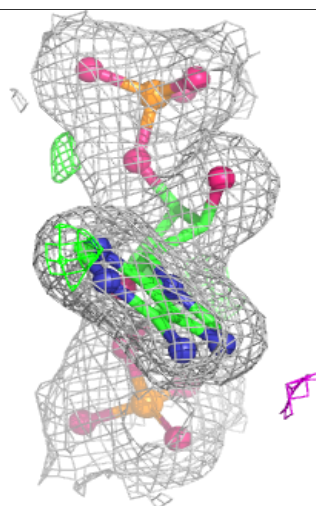
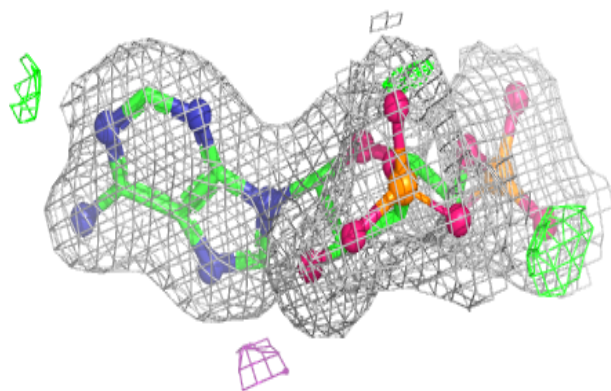
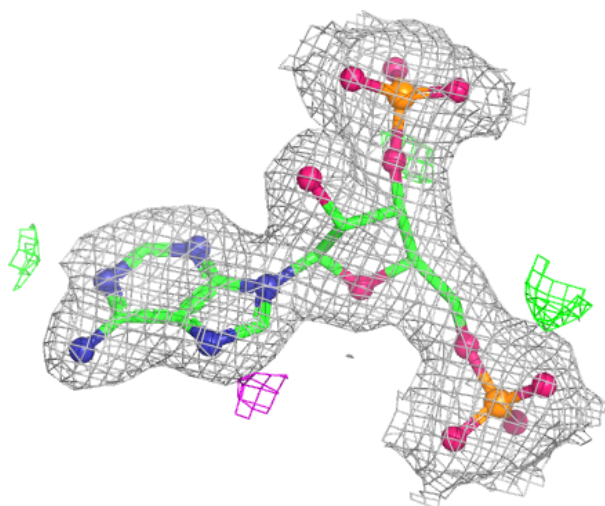
Electron density around A3P A 702:

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



Electron density around A3P 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.