



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 05:03 am BST

PDB ID : 6OHP
Title : Structure of compound 1 (halopemide) bound human Phospholipase D2 catalytic domain
Authors : Metrick, C.M.; Chodaparambil, J.V.
Deposited on : 2019-04-06
Resolution : 2.60 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 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 : 2.11
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) : 2.11

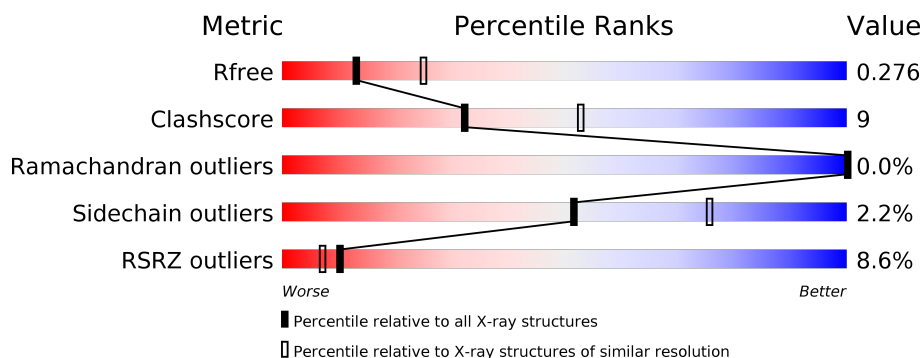
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	640	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>8%</div> </div> </div>
1	B	640	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>9%</div> </div> </div>
1	C	640	<div> <div>12%</div> <div> <div></div> <div>69%</div> <div>20%</div> <div>10%</div> </div> </div>
1	D	640	<div> <div>12%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>9%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PTR	C	573	-	-	-	X
1	PTR	D	573	-	-	-	X
3	SO4	B	1002	-	-	X	X
3	SO4	B	1003	-	-	X	-
3	SO4	B	1004	-	-	X	X

2 Entry composition [i](#)

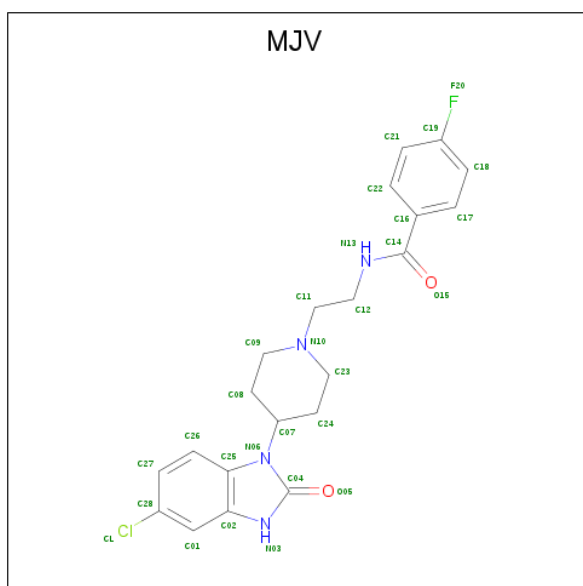
There are 5 unique types of molecules in this entry. The entry contains 19201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase D2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	586	Total	C	N	O	P	S	0	0	0
			4724	3030	827	850	1	16			
1	B	584	Total	C	N	O	P	S	0	0	0
			4714	3022	825	850	1	16			
1	C	579	Total	C	N	O	P	S	0	0	0
			4669	2994	818	840	1	16			
1	D	582	Total	C	N	O	P	S	0	0	0
			4690	3009	822	842	1	16			

- Molecule 2 is N-{2-[4-(5-chloro-2-oxo-2,3-dihydro-1H-benzimidazol-1-yl)piperidin-1-yl]ethyl}-4-fluorobenzamide (three-letter code: MJV) (formula: C₂₁H₂₂ClFN₄O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			29	21	1	1	4	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	F	N	O	0	0
			29	21	1	1	4	2		
2	C	1	Total	C	Cl	F	N	O	0	0
			29	21	1	1	4	2		
2	D	1	Total	C	Cl	F	N	O	0	0
			29	21	1	1	4	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

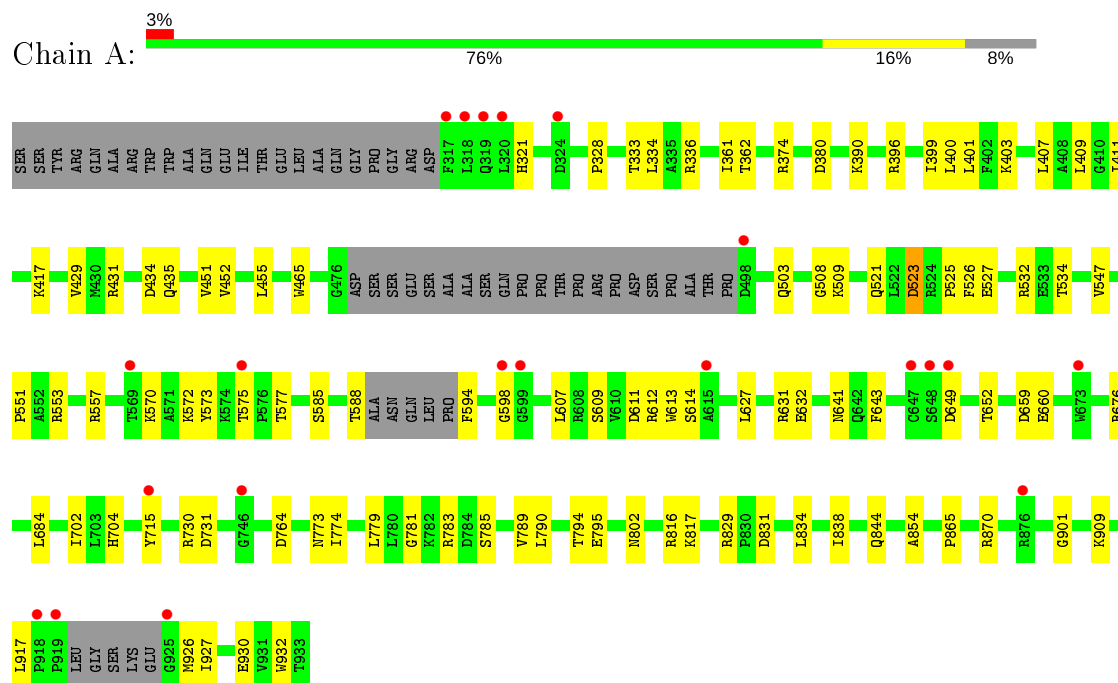
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	95	Total	O	0	0
			95	95		
5	B	83	Total	O	0	0
			83	83		
5	C	33	Total	O	0	0
			33	33		
5	D	34	Total	O	0	0
			34	34		

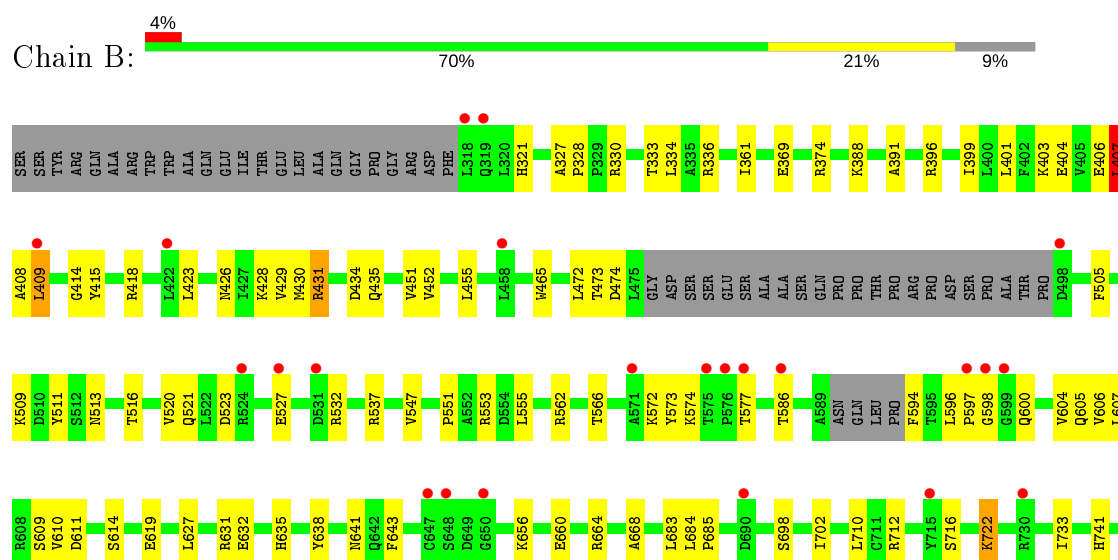
3 Residue-property plots [i](#)

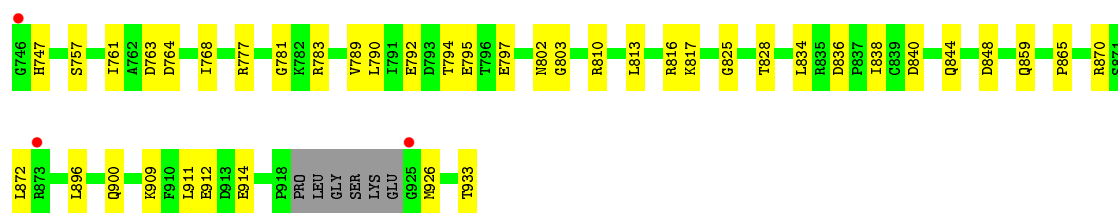
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phospholipase D2

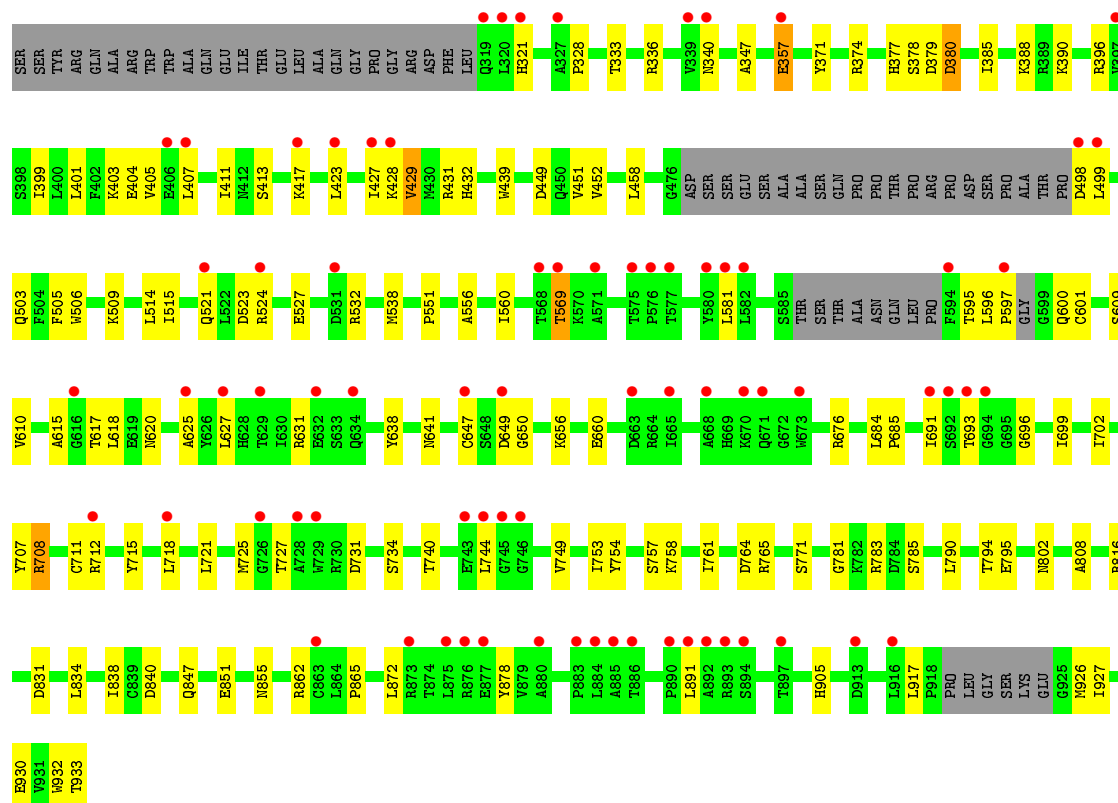


• Molecule 1: Phospholipase D2

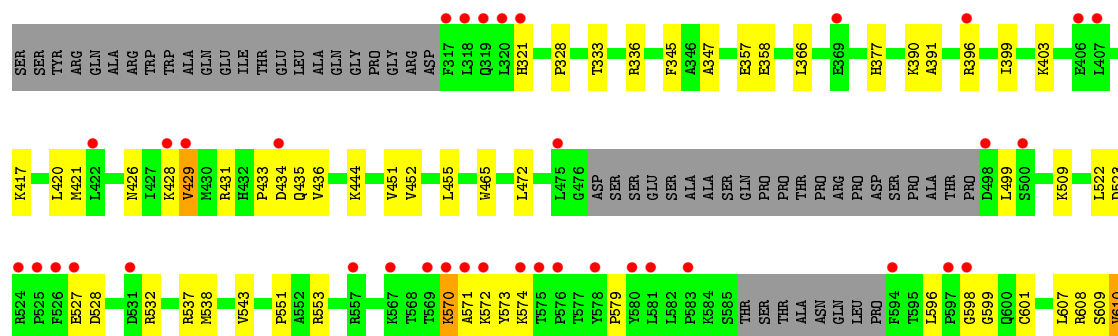
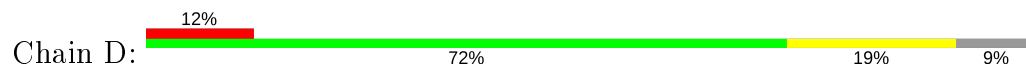


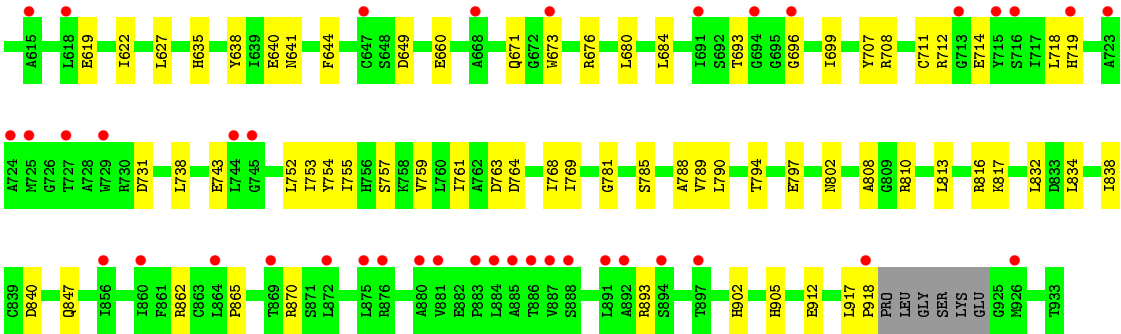


• Molecule 1: Phospholipase D2



• Molecule 1: Phospholipase D2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.19Å 132.51Å 114.64Å 90.00° 100.34° 90.00°	Depositor
Resolution (Å)	48.29 – 2.60 48.29 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.29-2.60) 99.5 (48.29-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13 _2998: ???)	Depositor
R, R_{free}	0.240 , 0.276 0.240 , 0.276	Depositor DCC
R_{free} test set	4008 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19201	wwPDB-VP
Average B, all atoms (Å ²)	57.0	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 57.44 % 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 2.3672e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MJV, SO4, PTR

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	0.26	0/4829	0.48	0/6562
1	B	0.26	0/4817	0.48	0/6545
1	C	0.26	0/4771	0.48	1/6483 (0.0%)
1	D	0.25	0/4794	0.46	0/6513
All	All	0.26	0/19211	0.47	1/26103 (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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	595	THR	C-N-CA	-5.91	106.94	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	408	ALA	Peptide
1	C	407	LEU	Peptide

5.2 Too-close contacts ⓘ

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	4724	0	4665	69	0
1	B	4714	0	4663	97	0
1	C	4669	0	4601	90	1
1	D	4690	0	4623	79	1
2	A	29	0	0	1	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	0	0
3	A	5	0	0	1	0
3	B	20	0	0	14	0
4	A	18	0	24	5	0
5	A	95	0	0	17	0
5	B	83	0	0	19	0
5	C	33	0	0	13	0
5	D	34	0	0	9	0
All	All	19201	0	18576	331	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 9.

All (331) 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:C:618:LEU:O	5:C:1101:HOH:O	1.86	0.93
1:B:712:ARG:NH1	5:B:1101:HOH:O	1.96	0.93
1:B:606:VAL:N	3:B:1003:SO4:O4	2.05	0.89
1:C:933:THR:O	5:C:1102:HOH:O	1.92	0.86
1:A:508:GLY:O	5:A:1101:HOH:O	1.92	0.86
1:C:783:ARG:NH1	5:C:1104:HOH:O	2.09	0.86
1:D:417:LYS:NZ	1:D:573:PTR:O1P	2.10	0.84
1:A:336:ARG:HD2	1:A:598:GLY:HA3	1.61	0.83
1:A:435:GLN:OE1	5:A:1102:HOH:O	1.96	0.83
1:A:575:THR:HG22	1:A:577:THR:H	1.44	0.82
1:A:901:GLY:O	5:A:1103:HOH:O	1.98	0.81
1:B:474:ASP:OD2	5:B:1102:HOH:O	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:GLN:NE2	1:B:632:GLU:OE1	2.16	0.79
1:C:340:ASN:O	5:C:1103:HOH:O	2.02	0.76
1:C:347:ALA:HB1	1:C:596:LEU:HD21	1.67	0.76
1:A:328:PRO:O	5:A:1104:HOH:O	2.03	0.75
1:B:872:LEU:HD23	1:B:914:GLU:HG3	1.69	0.75
1:D:444:LYS:O	5:D:1101:HOH:O	2.02	0.74
1:A:795:GLU:OE2	5:A:1105:HOH:O	2.05	0.74
1:B:933:THR:OG1	3:B:1002:SO4:O2	2.04	0.74
1:B:619:GLU:OE1	5:B:1103:HOH:O	2.05	0.74
1:C:734:SER:OG	1:C:847:GLN:NE2	2.21	0.73
1:A:417:LYS:NZ	1:A:429:VAL:O	2.20	0.73
1:A:553:ARG:NH1	1:A:585:SER:O	2.21	0.73
1:A:361:ILE:HB	1:A:399:ILE:HG23	1.71	0.73
1:C:862:ARG:NH2	1:C:878:TYR:O	2.21	0.73
1:C:631:ARG:NH1	5:C:1107:HOH:O	2.21	0.72
1:C:379:ASP:HB3	1:C:385:ILE:HD13	1.71	0.72
1:C:336:ARG:NH1	1:C:597:PRO:O	2.22	0.72
1:D:917:LEU:HD12	1:D:918:PRO:HD2	1.70	0.72
1:B:816:ARG:NH2	1:B:834:LEU:O	2.21	0.71
1:D:509:LYS:NZ	1:D:527:GLU:O	2.22	0.71
1:C:509:LYS:NZ	1:C:527:GLU:O	2.24	0.70
1:A:523:ASP:OD2	5:A:1106:HOH:O	2.10	0.69
1:B:840:ASP:OD1	5:B:1104:HOH:O	2.11	0.68
1:C:521:GLN:CG	1:C:524:ARG:HB2	2.23	0.68
1:C:521:GLN:HG2	1:C:524:ARG:HB2	1.74	0.68
1:B:361:ILE:HB	1:B:399:ILE:HG23	1.75	0.68
1:B:859:GLN:O	5:B:1105:HOH:O	2.12	0.68
1:B:574:LYS:O	5:B:1106:HOH:O	2.12	0.67
1:C:515:ILE:HG21	1:C:691:ILE:HD11	1.77	0.67
1:D:451:VAL:HG23	1:D:452:VAL:HG23	1.77	0.67
1:B:505:PHE:N	5:B:1102:HOH:O	2.28	0.67
1:B:792:GLU:OE2	5:B:1107:HOH:O	2.13	0.66
1:B:418:ARG:NH2	5:B:1113:HOH:O	2.27	0.66
1:A:380:ASP:O	5:A:1107:HOH:O	2.12	0.66
1:B:505:PHE:O	5:B:1108:HOH:O	2.14	0.65
1:B:473:THR:OG1	3:B:1004:SO4:O3	2.14	0.65
1:A:930:GLU:O	5:A:1109:HOH:O	2.14	0.65
1:A:816:ARG:NH2	1:A:834:LEU:O	2.26	0.65
1:D:601:CYS:SG	5:D:1103:HOH:O	2.55	0.65
1:D:433:PRO:HB2	1:D:435:GLN:HE21	1.60	0.64
1:D:571:ALA:HA	1:D:574:LYS:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:LEU:HB2	1:C:431:ARG:HG2	1.78	0.64
1:D:570:LYS:O	1:D:574:LYS:HG3	1.96	0.64
1:B:572:LYS:NZ	1:B:573:PTR:O2P	2.23	0.64
1:D:609:SER:OG	5:D:1102:HOH:O	2.15	0.64
1:D:794:THR:OG1	5:D:1103:HOH:O	2.15	0.63
1:C:707:TYR:HB3	1:C:712:ARG:HG3	1.79	0.63
1:A:926:MET:H	1:A:927:ILE:HD12	1.64	0.62
1:A:870:ARG:HE	1:A:909:LYS:HE2	1.63	0.62
1:C:521:GLN:HG3	1:C:524:ARG:NE	2.13	0.62
1:D:403:LYS:NZ	1:D:434:ASP:OD1	2.26	0.62
1:B:870:ARG:HE	1:B:909:LYS:HE2	1.65	0.61
1:C:506:TRP:O	1:C:532:ARG:NH2	2.28	0.61
1:C:816:ARG:NH2	1:C:834:LEU:O	2.31	0.61
1:D:847:GLN:OE1	1:D:905:HIS:NE2	2.28	0.61
1:A:409:LEU:HD22	1:A:411:ILE:HG12	1.82	0.61
1:B:605:GLN:HA	3:B:1003:SO4:O1	2.00	0.61
1:C:521:GLN:HG2	1:C:521:GLN:O	2.00	0.61
1:B:844:GLN:NE2	1:B:848:ASP:OD1	2.33	0.61
1:C:451:VAL:HG23	1:C:452:VAL:HG23	1.83	0.60
1:A:631:ARG:NH1	1:A:660:GLU:OE2	2.34	0.60
1:B:684:LEU:HG	1:B:865:PRO:HD3	1.82	0.60
1:B:396:ARG:HD3	5:B:1122:HOH:O	2.01	0.60
1:A:643:PHE:HA	4:A:1003:GOL:H32	1.83	0.60
1:B:330:ARG:HG2	3:B:1003:SO4:O1	2.01	0.60
1:A:396:ARG:O	5:A:1111:HOH:O	2.17	0.59
1:C:676:ARG:NH2	1:C:840:ASP:OD1	2.36	0.59
1:C:794:THR:OG1	5:C:1105:HOH:O	2.14	0.59
1:C:930:GLU:O	5:C:1104:HOH:O	2.16	0.58
1:B:783:ARG:NH1	3:B:1002:SO4:S	2.76	0.58
1:C:627:LEU:HB3	5:C:1107:HOH:O	2.03	0.58
1:D:336:ARG:HD3	1:D:598:GLY:HA3	1.85	0.58
1:C:521:GLN:HG3	1:C:524:ARG:HE	1.68	0.58
1:B:698:SER:O	1:B:702:ILE:HG22	2.04	0.58
1:B:777:ARG:N	3:B:1002:SO4:O1	2.37	0.57
1:B:609:SER:HB3	1:B:781:GLY:HA2	1.86	0.57
1:D:336:ARG:NH1	5:D:1110:HOH:O	2.37	0.57
1:B:797:GLU:HG3	1:B:810:ARG:HG2	1.86	0.57
1:D:609:SER:HB3	1:D:781:GLY:HA2	1.86	0.57
1:D:673:TRP:O	5:D:1104:HOH:O	2.16	0.57
1:C:413:SER:OG	1:C:431:ARG:NH1	2.38	0.56
1:C:515:ILE:HG21	1:C:691:ILE:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:SER:OG	1:C:380:ASP:OD2	2.23	0.56
1:B:404:GLU:HB2	1:B:409:LEU:HD23	1.87	0.56
1:C:696:GLY:H	1:C:699:ILE:HD13	1.69	0.56
1:A:333:THR:HG21	1:A:551:PRO:HG2	1.87	0.56
1:C:417:LYS:HG3	1:C:429:VAL:HG13	1.86	0.56
1:B:553:ARG:HD2	1:B:586:THR:HA	1.87	0.56
1:D:347:ALA:HB1	1:D:596:LEU:HD21	1.87	0.56
1:A:607:LEU:HD11	1:A:790:LEU:HB2	1.87	0.55
1:A:451:VAL:HG23	1:A:452:VAL:HG23	1.87	0.55
1:D:572:LYS:HE2	1:D:573:PTR:HE2	1.87	0.55
1:D:759:VAL:HG12	1:D:769:ILE:HG12	1.89	0.55
1:B:600:GLN:NE2	1:B:795:GLU:OE1	2.40	0.55
1:D:862:ARG:NE	5:D:1106:HOH:O	2.34	0.55
1:D:431:ARG:NH2	5:D:1111:HOH:O	2.40	0.55
1:A:844:GLN:NE2	3:A:1002:SO4:O3	2.33	0.54
1:B:406:GLU:O	1:B:407:LEU:HB2	2.07	0.54
1:B:511:TYR:CE2	1:B:537:ARG:HG3	2.42	0.54
1:A:508:GLY:H	4:A:1005:GOL:H12	1.71	0.54
1:D:676:ARG:NH2	1:D:840:ASP:OD1	2.40	0.54
1:D:649:ASP:HB3	1:D:708:ARG:HH12	1.73	0.54
1:B:643:PHE:CD1	1:B:702:ILE:HD11	2.43	0.54
1:C:610:VAL:HG11	1:C:615:ALA:HB3	1.90	0.53
1:B:414:GLY:HA2	1:B:431:ARG:HH12	1.73	0.53
1:B:455:LEU:HD11	1:B:789:VAL:HG13	1.89	0.53
1:C:684:LEU:HG	1:C:865:PRO:HD3	1.91	0.53
1:C:647:CYS:O	1:C:708:ARG:NH2	2.41	0.53
1:A:773:ASN:ND2	2:A:1001:MJV:O05	2.38	0.53
1:D:743:GLU:CD	1:D:893:ARG:HE	2.12	0.53
1:A:783:ARG:NH1	5:A:1109:HOH:O	2.40	0.53
1:A:794:THR:OG1	5:A:1110:HOH:O	2.14	0.53
1:B:327:ALA:HB1	3:B:1003:SO4:O2	2.09	0.53
1:A:844:GLN:HG3	1:B:631:ARG:HD2	1.91	0.53
1:D:366:LEU:HD22	1:D:420:LEU:HD11	1.90	0.53
1:A:612:ARG:NH1	5:A:1121:HOH:O	2.40	0.52
1:B:451:VAL:HG23	1:B:452:VAL:HG23	1.91	0.52
1:A:570:LYS:HE2	1:A:573:PTR:P	2.49	0.52
1:B:777:ARG:HB2	3:B:1002:SO4:O3	2.10	0.52
1:C:333:THR:HG21	1:C:551:PRO:HG2	1.92	0.52
1:C:625:ALA:HB1	1:C:790:LEU:HD12	1.91	0.52
1:B:783:ARG:HD3	3:B:1002:SO4:O4	2.09	0.52
1:C:609:SER:OG	5:C:1106:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:649:ASP:OD1	1:C:650:GLY:N	2.42	0.52
1:D:543:VAL:HG11	1:D:759:VAL:HG11	1.91	0.52
1:D:816:ARG:NH2	1:D:834:LEU:O	2.42	0.52
1:C:600:GLN:NE2	1:C:795:GLU:OE1	2.43	0.52
1:D:802:ASN:HB2	1:D:838:ILE:HD11	1.93	0.52
1:A:321:HIS:CD2	1:A:328:PRO:HB3	2.45	0.51
1:B:638:TYR:HB3	1:B:761:ILE:HB	1.92	0.51
1:A:401:LEU:HD13	1:A:429:VAL:HG13	1.92	0.51
1:A:779:LEU:O	5:A:1112:HOH:O	2.19	0.51
1:B:747:HIS:NE2	5:B:1117:HOH:O	2.34	0.51
1:C:802:ASN:HB2	1:C:838:ILE:HD11	1.91	0.51
1:D:428:LYS:HD3	1:D:579:PRO:HD2	1.93	0.51
1:C:509:LYS:HE3	1:C:521:GLN:HB3	1.93	0.51
1:D:753:ILE:O	5:D:1105:HOH:O	2.19	0.50
1:B:391:ALA:HB1	1:B:426:ASN:HB2	1.93	0.50
1:B:321:HIS:CD2	1:B:328:PRO:HB3	2.47	0.50
1:D:345:PHE:HD2	1:D:465:TRP:HD1	1.58	0.50
1:D:638:TYR:HB3	1:D:761:ILE:HB	1.93	0.50
1:D:764:ASP:HB3	1:D:808:ALA:HB1	1.92	0.50
1:B:401:LEU:HD13	1:B:429:VAL:HG13	1.93	0.50
1:C:676:ARG:NH1	1:C:731:ASP:O	2.42	0.50
1:D:377:HIS:HA	1:D:499:LEU:O	2.12	0.50
1:B:474:ASP:OD2	1:B:532:ARG:NH1	2.45	0.50
1:A:817:LYS:NZ	5:A:1116:HOH:O	2.29	0.49
1:C:423:LEU:HB2	1:C:427:ILE:HD12	1.93	0.49
1:D:336:ARG:HB2	1:D:599:GLY:HA2	1.94	0.49
1:B:403:LYS:NZ	1:B:434:ASP:OD2	2.39	0.49
1:C:374:ARG:HD3	1:C:505:PHE:O	2.11	0.49
1:D:711:CYS:HB3	1:D:718:LEU:HD12	1.95	0.49
1:B:430:MET:HE3	1:B:566:THR:HB	1.94	0.49
1:D:391:ALA:HB1	1:D:426:ASN:HB2	1.95	0.49
1:C:399:ILE:HB	1:C:429:VAL:HB	1.94	0.49
1:C:638:TYR:HB3	1:C:761:ILE:HB	1.93	0.49
1:D:451:VAL:HG12	1:D:553:ARG:HH21	1.77	0.49
1:A:594:PHE:N	5:A:1124:HOH:O	2.46	0.49
1:D:333:THR:HG21	1:D:551:PRO:HG2	1.94	0.48
1:D:640:GLU:HG3	1:D:680:LEU:HB3	1.94	0.48
1:C:388:LYS:HB2	1:C:423:LEU:HB3	1.96	0.48
1:C:357:GLU:HG3	1:C:449:ASP:OD1	2.13	0.48
1:B:611:ASP:H	1:B:614:SER:HG	1.61	0.48
1:B:414:GLY:HA2	1:B:431:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:LEU:HD11	1:B:790:LEU:HB2	1.96	0.48
1:C:764:ASP:HB3	1:C:808:ALA:HB1	1.94	0.48
1:D:696:GLY:H	1:D:699:ILE:HD13	1.78	0.48
1:D:538:MET:HE3	1:D:754:TYR:HB2	1.96	0.48
1:B:474:ASP:O	1:B:532:ARG:HD3	2.13	0.48
1:C:617:THR:OG1	5:C:1101:HOH:O	2.20	0.48
1:D:396:ARG:NH1	1:D:428:LYS:HE2	2.28	0.48
1:B:656:LYS:NZ	5:B:1128:HOH:O	2.46	0.48
1:C:428:LYS:HD3	1:C:428:LYS:HA	1.73	0.48
1:A:509:LYS:NZ	1:A:521:GLN:O	2.46	0.47
1:B:594:PHE:N	5:B:1130:HOH:O	2.47	0.47
1:C:371:TYR:HB2	1:C:374:ARG:HH12	1.78	0.47
1:B:794:THR:OG1	5:B:1109:HOH:O	2.18	0.47
1:C:556:ALA:O	1:C:560:ILE:HG12	2.14	0.47
1:C:377:HIS:HA	1:C:499:LEU:O	2.14	0.47
1:C:432:HIS:CD2	1:C:569:THR:HG21	2.49	0.47
1:C:631:ARG:NH1	1:C:660:GLU:OE2	2.47	0.47
1:A:702:ILE:HD13	1:A:932:TRP:HB3	1.96	0.47
1:A:676:ARG:NH1	1:A:731:ASP:O	2.42	0.47
1:B:722:LYS:HE2	1:B:722:LYS:HB2	1.69	0.47
1:B:870:ARG:HB3	1:B:912:GLU:HG2	1.97	0.47
1:D:426:ASN:O	1:D:428:LYS:NZ	2.48	0.47
1:C:609:SER:HB3	1:C:781:GLY:HA2	1.97	0.47
1:C:708:ARG:HH12	1:C:715:TYR:HB2	1.79	0.47
1:B:825:GLY:O	1:B:900:GLN:NE2	2.47	0.47
1:B:870:ARG:HD3	1:B:912:GLU:OE2	2.14	0.47
1:D:433:PRO:CB	1:D:435:GLN:HE21	2.25	0.46
1:A:652:THR:O	5:A:1114:HOH:O	2.21	0.46
1:C:371:TYR:HB2	1:C:374:ARG:NH1	2.30	0.46
1:A:508:GLY:N	4:A:1005:GOL:H12	2.29	0.46
1:A:455:LEU:HD11	1:A:789:VAL:HG13	1.97	0.46
1:A:588:THR:O	5:A:1113:HOH:O	2.20	0.46
1:B:656:LYS:NZ	5:B:1131:HOH:O	2.48	0.46
1:B:803:GLY:N	1:B:836:ASP:OD2	2.39	0.46
1:B:406:GLU:HG3	1:B:407:LEU:H	1.81	0.46
1:B:783:ARG:NH1	3:B:1002:SO4:O4	2.47	0.46
1:C:711:CYS:HB3	1:C:718:LEU:HD12	1.97	0.46
1:D:676:ARG:NH1	1:D:731:ASP:O	2.46	0.46
1:C:847:GLN:OE1	1:C:905:HIS:NE2	2.48	0.46
1:D:707:TYR:HB3	1:D:712:ARG:HG3	1.96	0.46
1:A:503:GLN:HG2	1:C:831:ASP:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:THR:HG21	1:B:551:PRO:HG2	1.98	0.46
1:C:538:MET:HE3	1:C:754:TYR:HB2	1.98	0.46
1:C:403:LYS:HG3	1:C:431:ARG:NH1	2.30	0.45
1:C:601:CYS:SG	5:C:1105:HOH:O	2.61	0.45
1:C:744:LEU:HB3	1:C:749:VAL:HG11	1.99	0.45
1:D:570:LYS:HE3	1:D:570:LYS:HB3	1.46	0.45
1:A:362:THR:HG22	1:A:400:LEU:HB2	1.98	0.45
1:C:851:GLU:HB2	1:C:905:HIS:CE1	2.51	0.45
1:D:635:HIS:N	1:D:763:ASP:OD2	2.43	0.45
1:B:374:ARG:HG3	1:B:465:TRP:CE2	2.51	0.45
1:A:434:ASP:OD2	1:A:570:LYS:HE3	2.17	0.45
1:B:641:ASN:HA	1:B:757:SER:O	2.17	0.45
1:A:403:LYS:HB2	1:A:431:ARG:HB3	1.98	0.45
1:A:802:ASN:HB2	1:A:838:ILE:HD11	1.99	0.45
1:C:764:ASP:OD1	1:C:816:ARG:HD3	2.16	0.45
1:A:572:LYS:NZ	1:A:573:PTR:O2P	2.49	0.45
1:A:764:ASP:OD1	1:A:816:ARG:HD3	2.17	0.45
1:B:509:LYS:NZ	1:B:521:GLN:O	2.49	0.45
1:B:610:VAL:HG22	1:B:619:GLU:HB3	1.99	0.45
1:C:560:ILE:HD12	1:C:581:LEU:HB3	1.96	0.45
1:C:439:TRP:CE2	1:C:783:ARG:HG2	2.52	0.45
1:B:627:LEU:HD22	1:B:660:GLU:HG3	1.98	0.45
1:B:802:ASN:HB2	1:B:838:ILE:HD11	1.98	0.45
1:D:572:LYS:HG2	1:D:573:PTR:HD2	1.98	0.45
1:D:813:LEU:HD11	1:D:817:LYS:HE3	1.99	0.45
1:C:390:LYS:HA	1:C:390:LYS:HD2	1.73	0.45
1:D:684:LEU:HG	1:D:865:PRO:HD3	1.97	0.45
1:D:390:LYS:HA	1:D:390:LYS:HD3	1.57	0.45
1:D:571:ALA:HA	1:D:574:LYS:CD	2.46	0.45
1:D:610:VAL:HG23	1:D:619:GLU:HB3	1.97	0.45
1:B:509:LYS:HE3	1:B:527:GLU:O	2.17	0.44
1:B:656:LYS:HE2	1:B:656:LYS:HB3	1.66	0.44
1:C:498:ASP:CG	1:C:499:LEU:H	2.20	0.44
1:C:609:SER:O	1:C:785:SER:HA	2.17	0.44
1:D:321:HIS:ND1	1:D:328:PRO:HB3	2.33	0.44
1:B:635:HIS:N	1:B:763:ASP:OD1	2.47	0.44
1:A:547:VAL:HG21	1:A:551:PRO:HB2	2.00	0.44
1:B:513:ASN:HB3	1:B:516:THR:HB	2.00	0.44
1:B:741:HIS:CD2	1:B:896:LEU:HD13	2.53	0.44
1:D:870:ARG:HB3	1:D:912:GLU:HG2	2.00	0.44
1:B:369:GLU:OE2	1:B:415:TYR:OH	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LYS:NZ	1:B:577:THR:O	2.38	0.44
1:B:555:LEU:HG	1:B:606:VAL:HG21	1.99	0.44
1:D:357:GLU:HG3	1:D:358:GLU:N	2.32	0.44
1:A:532:ARG:NH2	4:A:1005:GOL:H32	2.33	0.44
1:C:758:LYS:HD3	1:C:771:SER:HA	2.00	0.44
1:D:538:MET:HE3	1:D:752:LEU:HD11	1.99	0.44
1:A:390:LYS:HD2	1:A:390:LYS:HA	1.80	0.43
1:B:710:LEU:C	1:B:716:SER:HB2	2.39	0.43
1:A:704:HIS:CG	1:A:917:LEU:HG	2.53	0.43
1:B:562:ARG:HD2	5:B:1110:HOH:O	2.18	0.43
1:A:649:ASP:HA	1:A:715:TYR:CE1	2.54	0.43
1:B:813:LEU:HD11	1:B:817:LYS:HE3	2.00	0.43
1:A:831:ASP:HB3	1:C:503:GLN:HG2	2.00	0.43
1:A:829:ARG:NH1	1:A:831:ASP:OD2	2.51	0.43
1:C:627:LEU:HD22	1:C:660:GLU:HG3	2.00	0.43
1:C:702:ILE:HD13	1:C:932:TRP:HB3	2.01	0.43
1:D:627:LEU:HD22	1:D:660:GLU:HG3	2.00	0.43
1:D:738:LEU:HD22	1:D:902:HIS:HB2	2.01	0.43
1:A:609:SER:HB3	1:A:781:GLY:HA2	2.00	0.43
1:D:797:GLU:OE2	1:D:810:ARG:NH1	2.50	0.43
1:B:474:ASP:N	5:B:1114:HOH:O	2.28	0.43
1:B:683:LEU:HD13	5:B:1112:HOH:O	2.19	0.42
1:C:685:PRO:HD2	1:C:699:ILE:HG23	2.01	0.42
1:D:714:GLU:HA	1:D:719:HIS:ND1	2.34	0.42
1:D:455:LEU:HD11	1:D:789:VAL:HG13	2.01	0.42
1:A:684:LEU:HG	1:A:865:PRO:HD3	2.00	0.42
1:C:340:ASN:O	1:C:458:LEU:HD21	2.20	0.42
1:D:538:MET:CE	1:D:754:TYR:HB2	2.49	0.42
1:A:611:ASP:HB3	1:A:613:TRP:CD1	2.54	0.42
1:B:473:THR:OG1	3:B:1004:SO4:O4	2.37	0.42
1:A:627:LEU:HD22	1:A:660:GLU:HG3	2.01	0.42
1:D:607:LEU:HD11	1:D:790:LEU:HB2	2.01	0.42
1:A:509:LYS:HE3	1:A:527:GLU:O	2.20	0.42
1:C:699:ILE:HD12	1:C:699:ILE:H	1.85	0.42
1:A:641:ASN:ND2	1:A:774:ILE:HG13	2.35	0.42
1:B:764:ASP:OD1	1:B:816:ARG:HD3	2.20	0.42
1:D:435:GLN:H	1:D:435:GLN:CD	2.22	0.42
1:B:685:PRO:HG2	1:B:702:ILE:HG23	2.02	0.41
1:A:609:SER:O	1:A:785:SER:HA	2.19	0.41
1:B:664:ARG:HH12	1:B:668:ALA:HB2	1.86	0.41
1:C:656:LYS:HE3	1:C:656:LYS:HB2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:LEU:O	1:D:537:ARG:HG2	2.20	0.41
1:A:854:ALA:HA	4:A:1004:GOL:H2	2.03	0.41
1:D:528:ASP:OD2	1:D:532:ARG:HD2	2.20	0.41
1:C:404:GLU:HB3	1:C:411:ILE:HD11	2.03	0.41
1:C:514:LEU:HB2	1:C:538:MET:HE1	2.01	0.41
1:D:608:ARG:HG3	1:D:610:VAL:HG22	2.00	0.41
1:B:328:PRO:O	3:B:1003:SO4:O2	2.37	0.41
1:C:328:PRO:O	5:C:1108:HOH:O	2.22	0.41
1:D:522:LEU:HA	1:D:522:LEU:HD23	1.91	0.41
1:C:740:THR:HB	1:C:753:ILE:HD11	2.03	0.41
1:D:609:SER:O	1:D:785:SER:HA	2.21	0.41
1:A:374:ARG:HG3	1:A:465:TRP:CE2	2.56	0.41
1:B:472:LEU:N	3:B:1004:SO4:O1	2.53	0.41
1:D:641:ASN:HA	1:D:757:SER:O	2.21	0.41
1:D:768:ILE:HG12	1:D:790:LEU:HD13	2.03	0.41
1:B:388:LYS:HB2	1:B:423:LEU:HB3	2.03	0.41
1:C:641:ASN:HA	1:C:757:SER:O	2.21	0.41
1:B:596:LEU:HD13	1:B:597:PRO:HD2	2.03	0.40
1:B:768:ILE:HG12	1:B:790:LEU:HD13	2.03	0.40
1:D:699:ILE:HD12	1:D:699:ILE:H	1.86	0.40
1:B:872:LEU:HD22	1:B:911:LEU:HD22	2.03	0.40
1:C:321:HIS:ND1	1:C:328:PRO:HB3	2.36	0.40
1:C:399:ILE:O	1:C:429:VAL:HA	2.21	0.40
1:D:622:ILE:HG12	1:D:788:ALA:HB3	2.02	0.40
1:A:525:PRO:HG2	1:A:526:PHE:CD1	2.57	0.40
1:D:399:ILE:O	1:D:429:VAL:HA	2.21	0.40
1:A:611:ASP:H	1:A:614:SER:HG	1.69	0.40
1:B:336:ARG:HD2	1:B:598:GLY:HA3	2.02	0.40
1:B:547:VAL:HG11	1:B:604:VAL:HG11	2.04	0.40
1:C:374:ARG:NH1	5:C:1114:HOH:O	2.54	0.40
1:C:721:LEU:O	1:C:725:MET:HG2	2.21	0.40
1:D:680:LEU:HG	1:D:755:ILE:HD13	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:855:ASN:ND2	1:D:671:GLN:O[1_554]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	577/640 (90%)	556 (96%)	21 (4%)	0	100	100
1	B	575/640 (90%)	557 (97%)	17 (3%)	1 (0%)	47	71
1	C	568/640 (89%)	549 (97%)	19 (3%)	0	100	100
1	D	573/640 (90%)	553 (96%)	20 (4%)	0	100	100
All	All	2293/2560 (90%)	2215 (97%)	77 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	407	LEU

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	506/553 (92%)	498 (98%)	8 (2%)	62	82
1	B	506/553 (92%)	495 (98%)	11 (2%)	52	76
1	C	499/553 (90%)	482 (97%)	17 (3%)	37	63
1	D	500/553 (90%)	491 (98%)	9 (2%)	59	80
All	All	2011/2212 (91%)	1966 (98%)	45 (2%)	52	76

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

Mol	Chain	Res	Type
1	A	334	LEU
1	A	407	LEU
1	A	523	ASP
1	A	534	THR
1	A	557	ARG
1	A	632	GLU
1	A	659	ASP
1	A	730	ARG
1	B	334	LEU
1	B	407	LEU
1	B	409	LEU
1	B	431	ARG
1	B	435	GLN
1	B	520	VAL
1	B	523	ASP
1	B	722	LYS
1	B	733	ILE
1	B	828	THR
1	B	926	MET
1	C	357	GLU
1	C	380	ASP
1	C	396	ARG
1	C	405	VAL
1	C	429	VAL
1	C	523	ASP
1	C	569	THR
1	C	620	ASN
1	C	693	THR
1	C	708	ARG
1	C	727	THR
1	C	765	ARG
1	C	872	LEU
1	C	891	LEU
1	C	917	LEU
1	C	926	MET
1	C	927	ILE
1	D	421	MET
1	D	429	VAL
1	D	436	VAL
1	D	523	ASP
1	D	570	LYS
1	D	610	VAL
1	D	644	PHE

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Mol	Chain	Res	Type
1	D	693	THR
1	D	832	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	600	GLN
1	C	847	GLN
1	D	435	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	PTR	C	573	1	15,16,17	1.86	2 (13%)	19,22,24	1.08	1 (5%)
1	PTR	B	573	1	15,16,17	1.36	2 (13%)	19,22,24	0.80	0
1	PTR	D	573	1	15,16,17	1.36	2 (13%)	19,22,24	0.63	0
1	PTR	A	573	1	15,16,17	1.23	2 (13%)	19,22,24	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	573	1	-	3/10/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	B	573	1	-	2/10/11/13	0/1/1/1
1	PTR	D	573	1	-	2/10/11/13	0/1/1/1
1	PTR	A	573	1	-	3/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	573	PTR	OH-CZ	-5.81	1.27	1.40
1	D	573	PTR	OH-CZ	-4.01	1.31	1.40
1	A	573	PTR	OH-CZ	-3.70	1.32	1.40
1	B	573	PTR	OH-CZ	-3.46	1.32	1.40
1	B	573	PTR	P-OH	2.63	1.63	1.59
1	A	573	PTR	P-OH	2.53	1.63	1.59
1	C	573	PTR	P-O2P	-2.36	1.45	1.54
1	D	573	PTR	P-OH	2.25	1.62	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	573	PTR	O2P-P-OH	2.51	113.09	105.24

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	573	PTR	O-C-CA-CB
1	A	573	PTR	CZ-OH-P-O1P
1	D	573	PTR	CA-CB-CG-CD2
1	B	573	PTR	CA-CB-CG-CD1
1	B	573	PTR	CA-CB-CG-CD2
1	D	573	PTR	CA-CB-CG-CD1
1	A	573	PTR	CA-CB-CG-CD2
1	C	573	PTR	CA-CB-CG-CD2
1	C	573	PTR	CA-CB-CG-CD1
1	A	573	PTR	CA-CB-CG-CD1

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	573	PTR	1	0
1	D	573	PTR	3	0
1	A	573	PTR	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	MJV	D	1001	-	28,32,32	2.80	11 (39%)	36,45,45	1.60	9 (25%)
3	SO4	B	1004	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	B	1005	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	1005	-	5,5,5	0.87	0	5,5,5	1.08	1 (20%)
2	MJV	B	1001	-	28,32,32	2.68	11 (39%)	36,45,45	1.90	9 (25%)
2	MJV	A	1001	-	28,32,32	2.74	11 (39%)	36,45,45	1.87	10 (27%)
2	MJV	C	1001	-	28,32,32	2.78	10 (35%)	36,45,45	1.61	9 (25%)
4	GOL	A	1004	-	5,5,5	0.87	0	5,5,5	0.92	0
3	SO4	B	1002	-	4,4,4	0.23	0	6,6,6	0.22	0
3	SO4	A	1002	-	4,4,4	0.14	0	6,6,6	0.05	0
4	GOL	A	1003	-	5,5,5	0.80	0	5,5,5	1.16	1 (20%)
3	SO4	B	1003	-	4,4,4	0.33	0	6,6,6	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MJV	D	1001	-	-	2/10/24/24	0/4/4/4
4	GOL	A	1005	-	-	0/4/4/4	-
2	MJV	B	1001	-	-	3/10/24/24	0/4/4/4
2	MJV	A	1001	-	-	1/10/24/24	0/4/4/4
2	MJV	C	1001	-	-	0/10/24/24	0/4/4/4
4	GOL	A	1003	-	-	0/4/4/4	-
4	GOL	A	1004	-	-	2/4/4/4	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	MJV	C04-N03	9.39	1.44	1.34
2	A	1001	MJV	C04-N03	9.27	1.44	1.34
2	D	1001	MJV	C04-N03	9.18	1.44	1.34
2	B	1001	MJV	C04-N03	7.88	1.42	1.34
2	D	1001	MJV	C28-CL	6.27	1.88	1.74
2	C	1001	MJV	C28-CL	6.12	1.87	1.74
2	A	1001	MJV	C28-CL	5.89	1.87	1.74
2	B	1001	MJV	C28-CL	5.51	1.86	1.74
2	B	1001	MJV	C16-C14	4.94	1.60	1.50
2	D	1001	MJV	C16-C14	4.12	1.58	1.50
2	C	1001	MJV	C16-C14	3.95	1.58	1.50
2	A	1001	MJV	C16-C14	3.92	1.58	1.50
2	B	1001	MJV	C14-N13	3.66	1.41	1.33
2	B	1001	MJV	C26-C27	3.30	1.43	1.36
2	D	1001	MJV	C14-N13	3.30	1.41	1.33
2	C	1001	MJV	C14-N13	3.03	1.40	1.33
2	A	1001	MJV	C14-N13	2.92	1.40	1.33
2	A	1001	MJV	C26-C27	2.79	1.42	1.36
2	D	1001	MJV	C26-C27	2.79	1.42	1.36
2	C	1001	MJV	C26-C27	2.68	1.42	1.36
2	B	1001	MJV	C18-C19	2.47	1.41	1.37
2	A	1001	MJV	C21-C19	2.40	1.41	1.37
2	D	1001	MJV	C18-C19	2.39	1.41	1.37
2	B	1001	MJV	C21-C19	2.36	1.41	1.37
2	D	1001	MJV	C01-C28	2.31	1.41	1.36
2	A	1001	MJV	C01-C28	2.31	1.41	1.36
2	C	1001	MJV	C01-C28	2.29	1.41	1.36
2	B	1001	MJV	C17-C16	2.29	1.43	1.39
2	B	1001	MJV	C18-C17	2.29	1.42	1.38
2	C	1001	MJV	C21-C19	2.25	1.41	1.37
2	D	1001	MJV	C01-C02	2.25	1.45	1.41
2	A	1001	MJV	C18-C19	2.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	MJV	C18-C19	2.21	1.41	1.37
2	B	1001	MJV	C26-C25	2.20	1.45	1.41
2	C	1001	MJV	C01-C02	2.15	1.45	1.41
2	D	1001	MJV	C02-N03	2.14	1.45	1.38
2	D	1001	MJV	C21-C19	2.14	1.41	1.37
2	C	1001	MJV	C02-N03	2.12	1.45	1.38
2	A	1001	MJV	C02-N03	2.12	1.45	1.38
2	A	1001	MJV	C22-C21	2.12	1.42	1.38
2	D	1001	MJV	C18-C17	2.11	1.42	1.38
2	A	1001	MJV	C01-C02	2.06	1.45	1.41
2	B	1001	MJV	C22-C21	2.05	1.42	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	MJV	C11-N10-C23	-4.73	99.14	111.23
2	A	1001	MJV	C09-C08-C07	4.19	113.72	110.44
2	B	1001	MJV	C23-C24-C07	-3.81	107.46	110.44
2	B	1001	MJV	C16-C14-N13	3.46	124.52	117.09
2	B	1001	MJV	C11-N10-C09	-3.46	102.39	111.23
2	A	1001	MJV	C08-C09-N10	3.40	116.39	111.11
2	B	1001	MJV	C04-N03-C02	3.26	110.24	103.78
2	A	1001	MJV	C16-C14-N13	3.15	123.86	117.09
2	C	1001	MJV	C04-N03-C02	3.14	110.00	103.78
2	A	1001	MJV	C04-N03-C02	3.11	109.96	103.78
2	D	1001	MJV	C04-N03-C02	3.08	109.89	103.78
2	A	1001	MJV	C23-N10-C09	2.95	115.47	108.83
2	C	1001	MJV	C16-C14-N13	2.90	123.32	117.09
2	D	1001	MJV	C23-C24-C07	-2.66	108.36	110.44
2	C	1001	MJV	C11-N10-C23	-2.60	104.58	111.23
2	C	1001	MJV	C23-N10-C09	2.47	114.39	108.83
2	D	1001	MJV	C11-N10-C23	-2.40	105.09	111.23
2	A	1001	MJV	C11-N10-C09	-2.40	105.10	111.23
2	D	1001	MJV	C23-N10-C09	2.35	114.11	108.83
2	A	1001	MJV	C24-C23-N10	2.35	114.75	111.11
2	A	1001	MJV	C21-C19-C18	-2.33	119.73	122.83
2	B	1001	MJV	C21-C19-C18	-2.32	119.74	122.83
2	D	1001	MJV	C16-C14-N13	2.32	122.08	117.09
2	B	1001	MJV	O15-C14-N13	-2.30	118.02	122.61
2	A	1001	MJV	O15-C14-N13	-2.27	118.08	122.61
2	D	1001	MJV	C21-C19-C18	-2.24	119.84	122.83
2	C	1001	MJV	C11-N10-C09	-2.24	105.50	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	MJV	C21-C19-C18	-2.23	119.86	122.83
2	B	1001	MJV	C08-C09-N10	2.23	114.57	111.11
2	D	1001	MJV	C08-C09-N10	2.22	114.56	111.11
2	D	1001	MJV	C24-C23-N10	2.18	114.50	111.11
4	A	1003	GOL	C3-C2-C1	-2.17	103.29	111.70
2	C	1001	MJV	O15-C14-N13	-2.13	118.36	122.61
2	B	1001	MJV	C12-N13-C14	2.09	126.86	122.08
2	D	1001	MJV	C01-C02-C25	-2.09	118.96	121.10
2	C	1001	MJV	C08-C09-N10	2.07	114.33	111.11
4	A	1005	GOL	C3-C2-C1	-2.05	103.73	111.70
2	C	1001	MJV	C01-C02-C25	-2.04	119.01	121.10
2	A	1001	MJV	C12-C11-N10	-2.03	107.82	112.88

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1001	MJV	N10-C11-C12-N13
2	D	1001	MJV	C12-C11-N10-C09
2	B	1001	MJV	N10-C11-C12-N13
2	B	1001	MJV	C12-C11-N10-C09
4	A	1004	GOL	O1-C1-C2-O2
4	A	1004	GOL	O1-C1-C2-C3
2	A	1001	MJV	C12-C11-N10-C09
2	B	1001	MJV	C12-C11-N10-C23

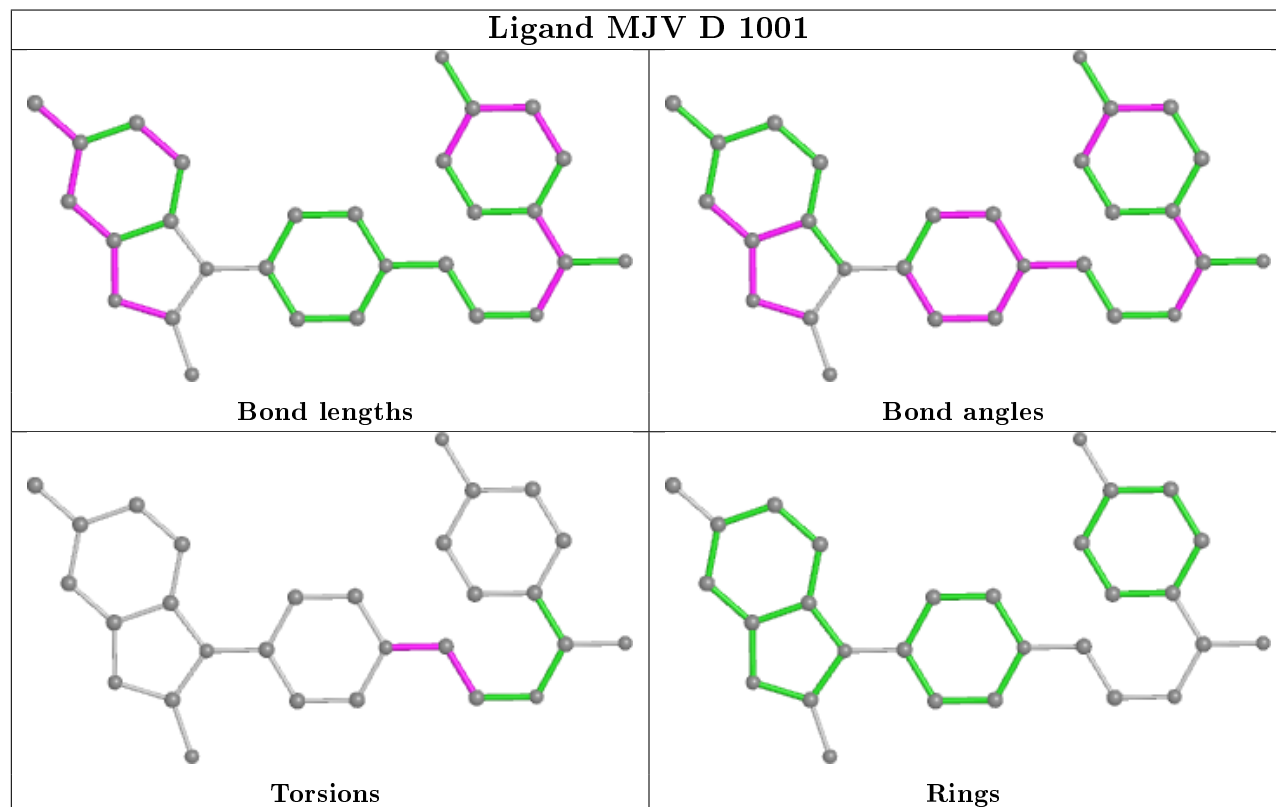
There are no ring outliers.

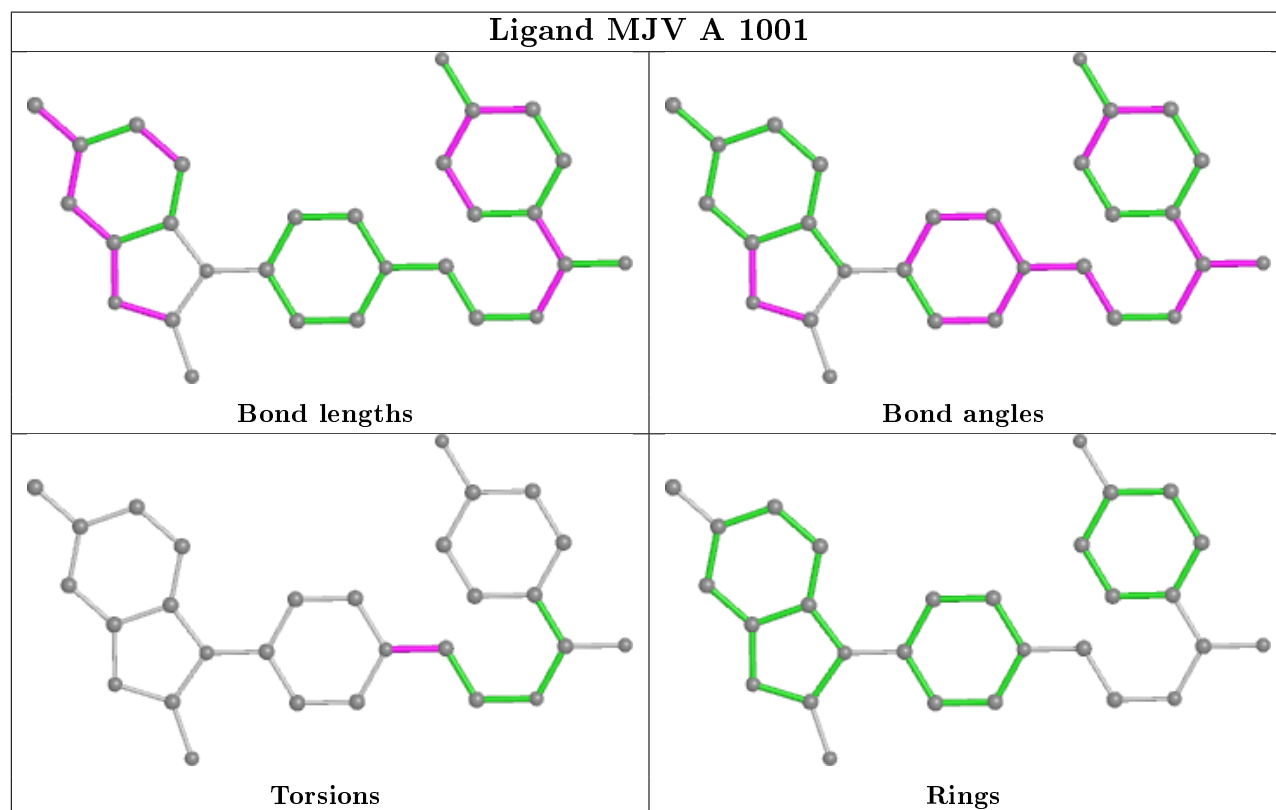
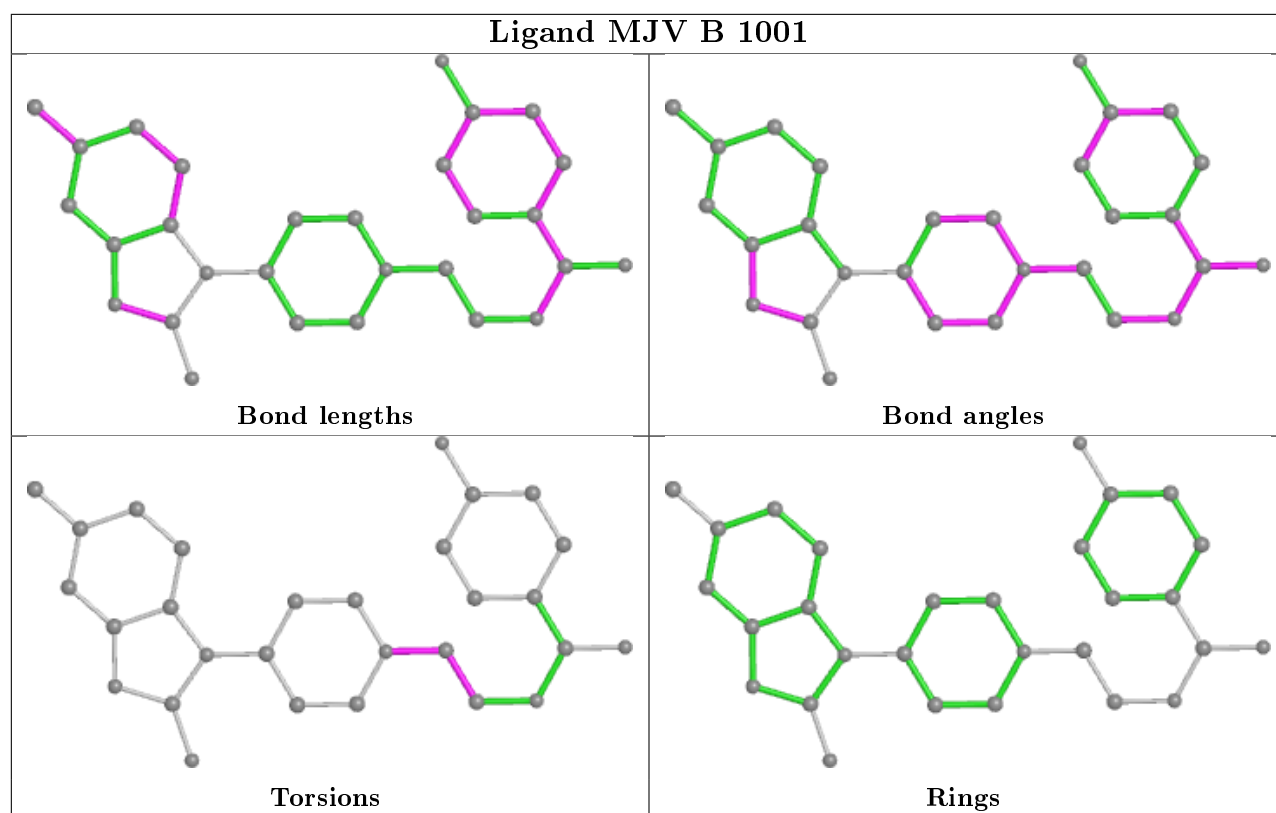
8 monomers are involved in 21 short contacts:

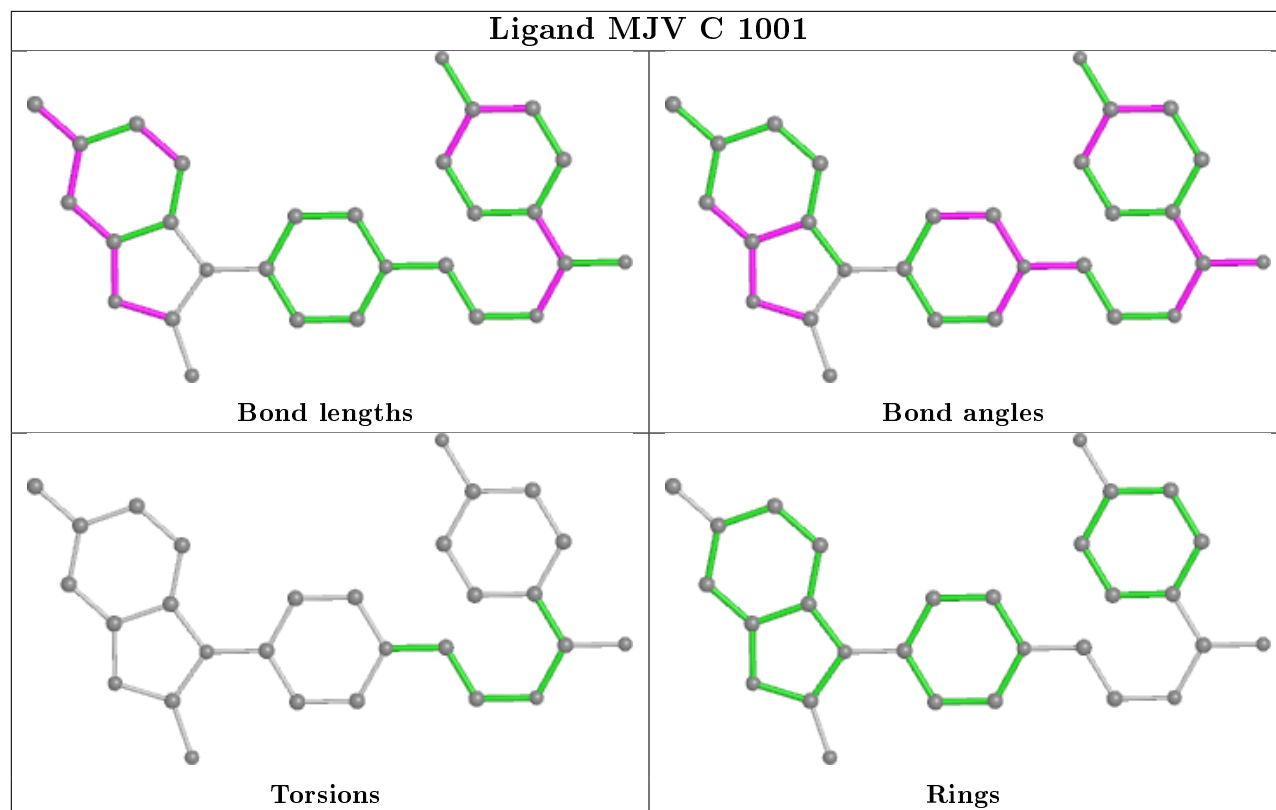
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1004	SO4	3	0
4	A	1005	GOL	3	0
2	A	1001	MJV	1	0
4	A	1004	GOL	1	0
3	B	1002	SO4	6	0
3	A	1002	SO4	1	0
4	A	1003	GOL	1	0
3	B	1003	SO4	5	0

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 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.







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, 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	585/640 (91%)	0.25	21 (3%) 42 35	26, 44, 72, 117	0
1	B	583/640 (91%)	0.36	26 (4%) 33 26	27, 45, 75, 97	0
1	C	578/640 (90%)	0.78	75 (12%) 3 2	42, 66, 98, 114	0
1	D	581/640 (90%)	0.87	77 (13%) 3 2	37, 64, 97, 128	0
All	All	2327/2560 (90%)	0.56	199 (8%) 10 7	26, 55, 92, 128	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	318	LEU	15.0
1	D	319	GLN	10.6
1	A	318	LEU	9.4
1	D	317	PHE	8.8
1	D	880	ALA	8.3
1	D	576	PRO	6.4
1	C	569	THR	6.1
1	D	571	ALA	5.9
1	A	319	GLN	5.8
1	D	891	LEU	5.7
1	D	570	LYS	5.5
1	D	598	GLY	5.4
1	D	744	LEU	5.3
1	D	569	THR	5.3
1	C	886	THR	5.2
1	D	428	LYS	5.1
1	C	319	GLN	5.0
1	D	892	ALA	4.9
1	D	580	TYR	4.9
1	D	574	LYS	4.6
1	C	597	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	746	GLY	4.5
1	C	498	ASP	4.4
1	D	888	SER	4.3
1	C	594	PHE	4.3
1	C	744	LEU	4.3
1	C	576	PRO	4.2
1	C	880	ALA	4.2
1	C	877	GLU	4.2
1	D	691	ILE	4.1
1	D	320	LEU	4.1
1	C	726	GLY	4.1
1	C	876	ARG	4.0
1	B	650	GLY	4.0
1	C	616	GLY	3.9
1	B	576	PRO	3.9
1	C	580	TYR	3.9
1	C	524	ARG	3.9
1	D	715	TYR	3.8
1	A	598	GLY	3.8
1	C	885	ALA	3.8
1	D	875	LEU	3.7
1	D	887	VAL	3.7
1	C	873	ARG	3.7
1	C	745	GLY	3.7
1	D	713	GLY	3.7
1	A	317	PHE	3.6
1	C	875	LEU	3.6
1	D	876	ARG	3.6
1	C	892	ALA	3.6
1	D	647	CYS	3.6
1	D	526	PHE	3.6
1	C	728	ALA	3.5
1	D	926	MET	3.5
1	B	575	THR	3.5
1	A	498	ASP	3.4
1	D	864	LEU	3.4
1	C	575	THR	3.4
1	B	597	PRO	3.4
1	C	691	ILE	3.3
1	C	890	PRO	3.3
1	C	581	LEU	3.3
1	C	634	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	885	ALA	3.3
1	A	647	CYS	3.3
1	D	498	ASP	3.3
1	D	884	LEU	3.3
1	D	860	ILE	3.2
1	A	649	ASP	3.2
1	B	531	ASP	3.2
1	D	886	THR	3.2
1	C	663	ASP	3.2
1	C	665	ILE	3.2
1	B	318	LEU	3.2
1	C	417	LYS	3.2
1	A	569	THR	3.1
1	C	407	LEU	3.1
1	C	884	LEU	3.1
1	B	598	GLY	3.1
1	B	571	ALA	3.1
1	D	575	THR	3.1
1	D	524	ARG	3.1
1	D	597	PRO	3.0
1	B	647	CYS	3.0
1	C	897	THR	3.0
1	D	531	ASP	3.0
1	D	567	LYS	2.9
1	A	715	TYR	2.9
1	C	883	PRO	2.9
1	C	712	ARG	2.9
1	B	319	GLN	2.9
1	C	627	LEU	2.9
1	D	578	TYR	2.9
1	C	673	TRP	2.8
1	C	397	VAL	2.8
1	D	881	VAL	2.8
1	A	919	PRO	2.8
1	C	327	ALA	2.8
1	D	723	ALA	2.8
1	B	715	TYR	2.8
1	C	427	ILE	2.8
1	D	745	GLY	2.8
1	A	320	LEU	2.8
1	A	673	TRP	2.8
1	D	527	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	320	LEU	2.8
1	D	727	THR	2.8
1	D	719	HIS	2.8
1	D	918	PRO	2.7
1	C	568	THR	2.7
1	C	647	CYS	2.7
1	A	876	ARG	2.7
1	C	668	ALA	2.7
1	D	883	PRO	2.7
1	C	694	GLY	2.7
1	D	406	GLU	2.7
1	D	615	ALA	2.7
1	D	422	LEU	2.7
1	D	897	THR	2.6
1	D	407	LEU	2.6
1	D	572	LYS	2.6
1	D	581	LEU	2.6
1	D	429	VAL	2.6
1	C	499	LEU	2.6
1	C	582	LEU	2.5
1	D	557	ARG	2.5
1	D	594	PHE	2.5
1	C	670	LYS	2.5
1	C	521	GLN	2.5
1	A	324	ASP	2.5
1	D	618	LEU	2.5
1	B	498	ASP	2.5
1	C	577	THR	2.5
1	C	632	GLU	2.5
1	B	873	ARG	2.5
1	C	671	GLN	2.5
1	A	918	PRO	2.4
1	D	729	TRP	2.4
1	D	894	SER	2.4
1	D	694	GLY	2.4
1	D	668	ALA	2.4
1	C	649	ASP	2.4
1	D	369	GLU	2.4
1	C	423	LEU	2.4
1	C	531	ASP	2.3
1	D	869	THR	2.3
1	B	524	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	583	PRO	2.3
1	A	599	GLY	2.3
1	D	724	ALA	2.3
1	A	648	SER	2.3
1	D	321	HIS	2.3
1	D	872	LEU	2.3
1	B	586	THR	2.3
1	C	692	SER	2.3
1	A	746	GLY	2.2
1	C	321	HIS	2.2
1	C	357	GLU	2.2
1	C	571	ALA	2.2
1	D	396	ARG	2.2
1	B	746	GLY	2.2
1	D	856	ILE	2.2
1	C	743	GLU	2.2
1	D	500	SER	2.2
1	B	409	LEU	2.2
1	B	422	LEU	2.2
1	A	615	ALA	2.2
1	C	625	ALA	2.2
1	C	894	SER	2.2
1	C	891	LEU	2.2
1	C	916	LEU	2.2
1	D	725	MET	2.2
1	B	648	SER	2.1
1	C	718	LEU	2.1
1	D	525	PRO	2.1
1	C	406	GLU	2.1
1	C	863	CYS	2.1
1	C	893	ARG	2.1
1	B	599	GLY	2.1
1	C	729	TRP	2.1
1	D	673	TRP	2.1
1	C	428	LYS	2.0
1	C	339	VAL	2.0
1	B	577	THR	2.0
1	B	925	GLY	2.0
1	C	693	THR	2.0
1	B	730	ARG	2.0
1	C	340	ASN	2.0
1	A	575	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	925	GLY	2.0
1	D	434	ASP	2.0
1	B	458	LEU	2.0
1	B	527	GLU	2.0
1	B	690	ASP	2.0
1	C	913	ASP	2.0
1	D	696	GLY	2.0
1	D	716	SER	2.0
1	C	629	THR	2.0
1	D	475	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PTR	C	573	16/17	0.56	0.41	100,103,110,115	0
1	PTR	D	573	16/17	0.61	0.42	100,104,111,117	0
1	PTR	A	573	16/17	0.73	0.24	65,70,80,88	0
1	PTR	B	573	16/17	0.74	0.25	61,69,81,83	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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	SO4	B	1004	5/5	0.34	0.60	112,148,160,160	0
2	MJV	D	1001	29/29	0.77	0.35	53,70,90,100	0
3	SO4	B	1002	5/5	0.80	0.66	124,154,162,169	0
3	SO4	A	1002	5/5	0.81	0.20	138,139,140,140	0

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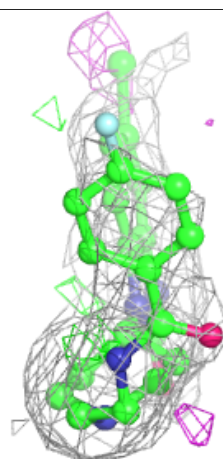
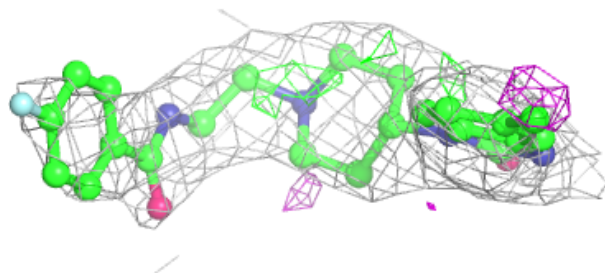
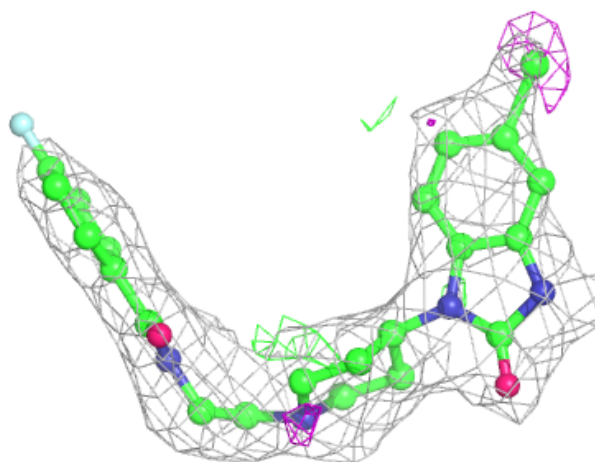
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MJV	C	1001	29/29	0.83	0.27	43,62,71,89	0
2	MJV	B	1001	29/29	0.87	0.27	38,44,51,60	0
3	SO4	B	1003	5/5	0.87	0.52	90,133,146,150	0
4	GOL	A	1004	6/6	0.89	0.38	56,58,61,62	0
2	MJV	A	1001	29/29	0.89	0.26	33,43,49,59	0
3	SO4	B	1005	5/5	0.90	0.29	148,149,149,153	0
4	GOL	A	1003	6/6	0.92	0.33	60,63,73,79	0
4	GOL	A	1005	6/6	0.92	0.33	66,67,71,76	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.

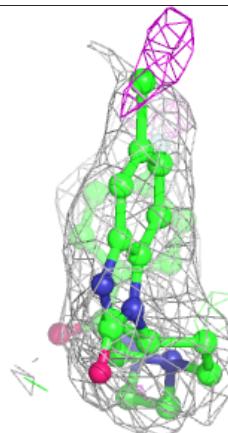
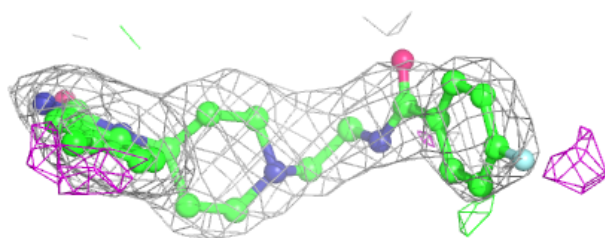
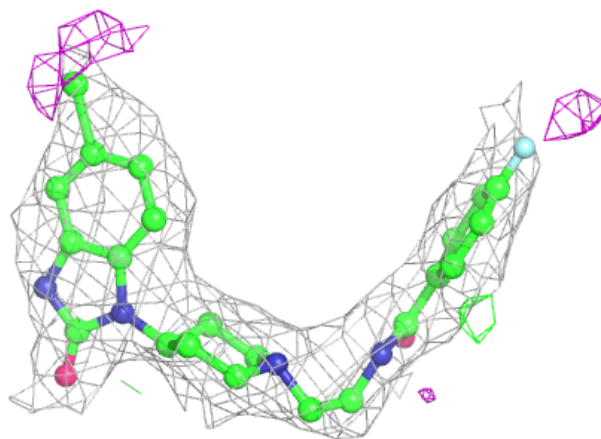
Electron density around MJV D 1001:

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



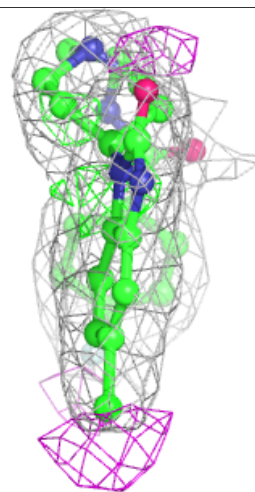
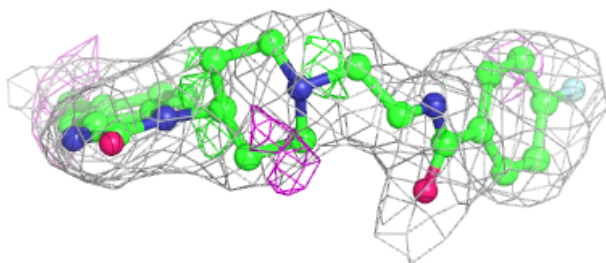
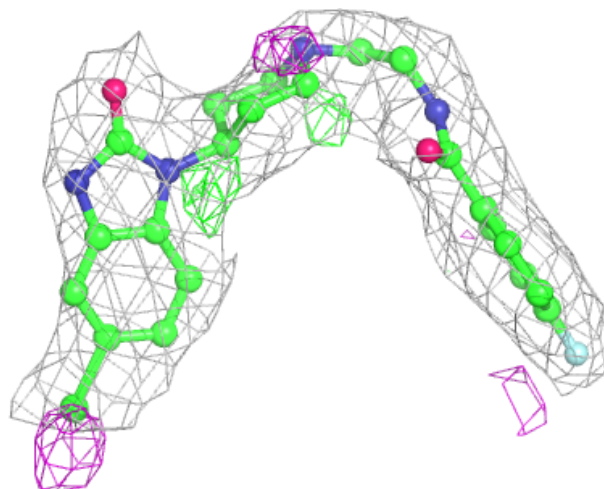
Electron density around MJV C 1001:

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



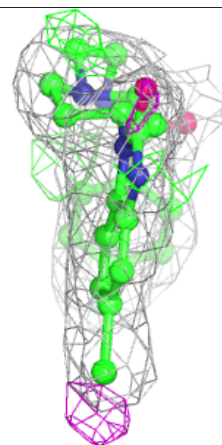
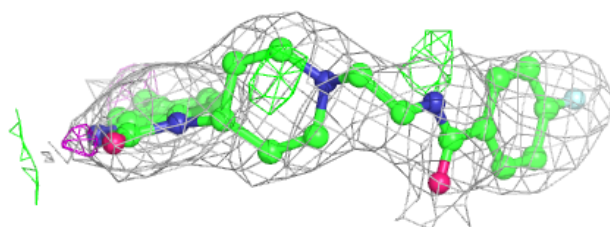
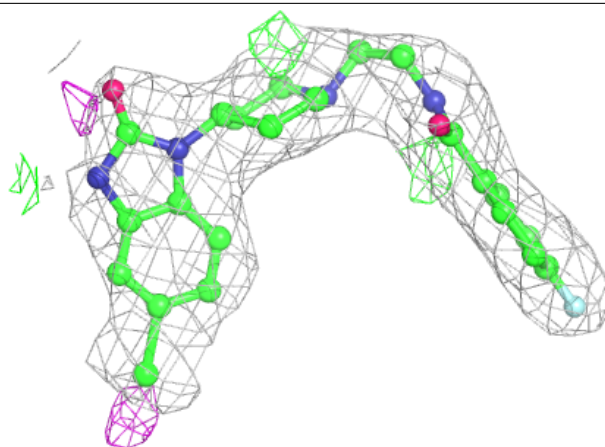
Electron density around MJV B 1001:

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



Electron density around MJV A 1001:

$2mF_o - DF_c$ (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.