



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:24 AM UTC

PDB ID : 2BED / pdb\_00002bed  
Title : Structure of FPT bound to inhibitor SCH207736  
Authors : Strickland, C.  
Deposited on : 2005-10-24  
Resolution : 2.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

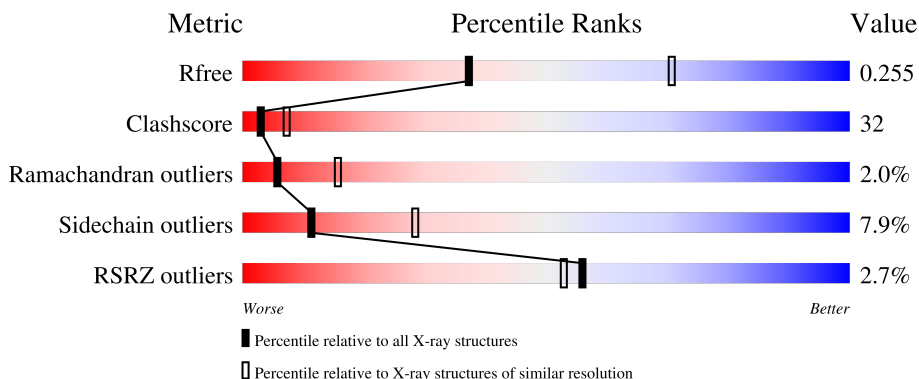
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

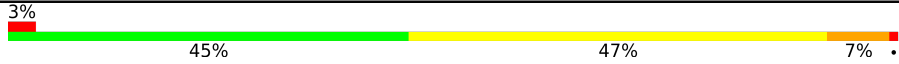
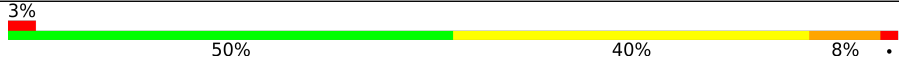
The reported resolution of this entry is 2.70 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	313	
2	B	401	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6264 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 Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	313	2665	1697	466	497	5	0	0	0

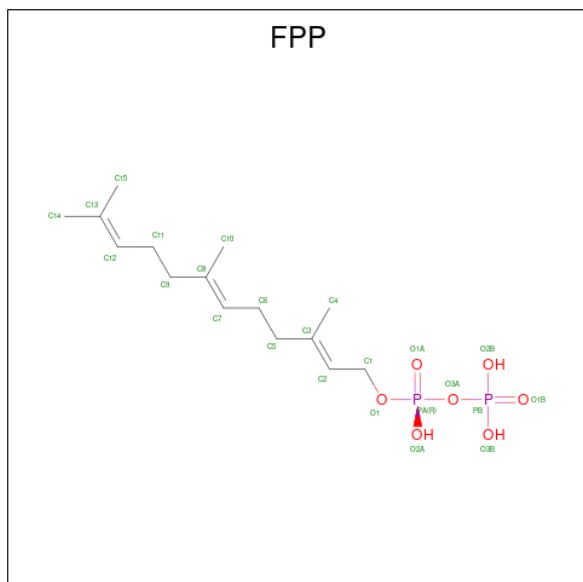
- Molecule 2 is a protein called Protein farnesyltransferase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	401	3154	2016	543	572	23	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

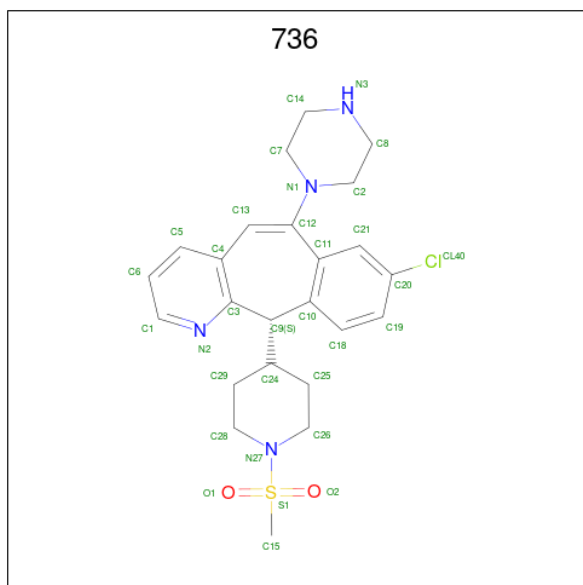
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is FARNESYL DIPHOSPHATE (CCD ID: FPP) (formula: C<sub>15</sub>H<sub>28</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
4	B	1	24	15	7	2	0	0

- Molecule 5 is (11S)-8-CHLORO-11-[1-(METHYLSULFONYL)PIPERIDIN-4-YL]-6-PIPERAZIN-1-YL-11H-BENZO[5,6]CYCLOHEPTA[1,2-B]PYRIDINE (CCD ID: 736) (formula:  $C_{24}H_{29}ClN_4O_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
5	B	1	32	24	1	4	2	1	0	0

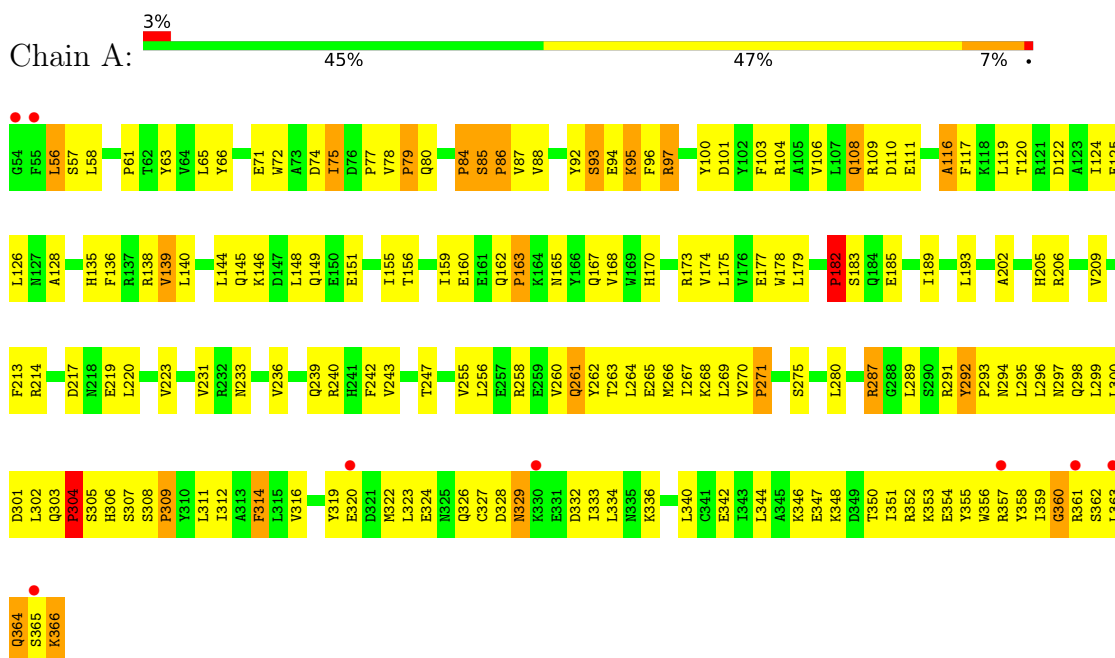
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	215	215	215	0	0
6	B	173	173	173	0	0

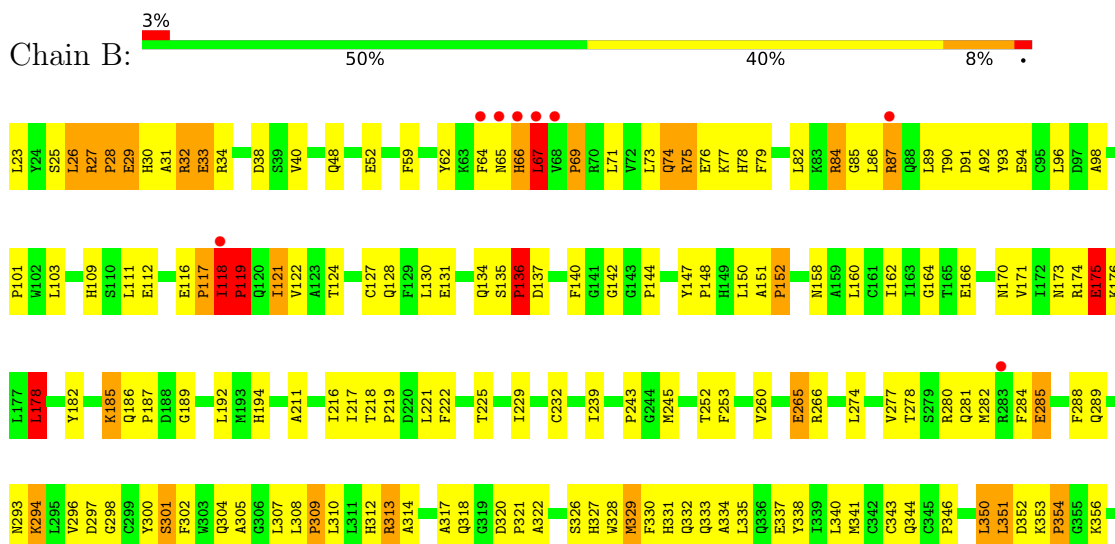
### 3 Residue-property plots

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: Protein farnesyltransferase/geranylgeranyltransferase type I alpha subunit



- Molecule 2: Protein farnesyltransferase beta subunit





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.02Å 174.02Å 69.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.70) 98.2 (50.00-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.72Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.223 , 0.262 0.218 , 0.255	Depositor DCC
$R_{free}$ test set	1662 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.8	Xtrriage
Anisotropy	0.093	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 736, FPP, ZN

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	0.45	0/2730	1.19	27/3705 (0.7%)
2	B	0.46	0/3239	1.14	29/4397 (0.7%)
All	All	0.45	0/5969	1.16	56/8102 (0.7%)

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	GLN	CA-C-N	11.88	132.23	119.87
1	A	162	GLN	C-N-CA	11.88	132.23	119.87
1	A	93	SER	N-CA-C	-9.58	98.31	110.19
1	A	75	ILE	N-CA-C	8.26	119.73	108.17
2	B	67	LEU	N-CA-C	7.82	121.20	109.95
1	A	350	THR	N-CA-C	7.33	120.32	111.82
1	A	348	LYS	N-CA-C	7.28	120.14	111.33
2	B	417	GLN	N-CA-C	-7.28	103.38	111.82
2	B	294	LYS	N-CA-C	-7.25	98.39	109.41
2	B	312	HIS	N-CA-C	-7.14	103.43	111.14
1	A	292	TYR	CA-C-N	6.77	127.04	119.32
1	A	292	TYR	C-N-CA	6.77	127.04	119.32
2	B	136	PRO	N-CA-C	-6.71	107.70	114.68
2	B	77	LYS	N-CA-C	6.67	118.63	111.36
1	A	97	ARG	N-CA-C	-6.46	104.15	111.07
1	A	364	GLN	N-CA-C	-6.22	105.70	113.28
2	B	245	MET	N-CA-C	6.05	119.47	110.52
1	A	270	VAL	CA-C-N	6.04	127.39	119.84
1	A	270	VAL	C-N-CA	6.04	127.39	119.84
2	B	175	GLU	N-CA-C	6.00	118.59	111.33
2	B	178	LEU	N-CA-C	-5.97	104.70	111.14
1	A	139	VAL	N-CA-C	-5.94	103.97	112.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	261	GLN	N-CA-C	-5.94	104.73	111.14
1	A	85	SER	CA-C-N	5.85	127.16	119.84
1	A	85	SER	C-N-CA	5.85	127.16	119.84
2	B	351	LEU	N-CA-C	5.84	117.13	108.60
1	A	314	PHE	N-CA-C	-5.71	105.14	111.36
1	A	100	TYR	N-CA-C	5.69	118.42	111.82
2	B	298	GLY	N-CA-C	5.69	119.77	112.83
1	A	149	GLN	N-CA-C	-5.69	105.22	111.82
2	B	75	ARG	N-CA-C	5.66	117.90	111.11
1	A	183	SER	N-CA-C	5.64	118.20	111.71
2	B	320	ASP	CA-C-N	5.60	125.30	119.64
2	B	320	ASP	C-N-CA	5.60	125.30	119.64
1	A	214	ARG	N-CA-CB	-5.55	102.96	111.74
2	B	192	LEU	N-CA-C	-5.54	102.33	110.52
2	B	381	MET	N-CA-C	5.45	118.13	109.96
1	A	163	PRO	N-CA-C	5.41	120.69	114.03
2	B	301	SER	N-CA-C	-5.39	105.97	112.54
2	B	32	ARG	N-CA-CB	-5.38	101.18	110.32
2	B	150	LEU	N-CA-C	5.34	117.79	111.33
2	B	66	HIS	CB-CA-C	-5.34	108.75	116.54
2	B	33	GLU	N-CA-C	-5.32	105.49	112.72
1	A	347	GLU	N-CA-C	5.30	119.24	111.34
2	B	32	ARG	CG-CD-NE	5.25	123.54	112.00
1	A	57	SER	N-CA-C	5.20	117.89	110.24
2	B	27	ARG	CA-C-N	5.18	126.31	119.84
2	B	27	ARG	C-N-CA	5.18	126.31	119.84
1	A	116	ALA	N-CA-C	-5.16	105.66	111.28
1	A	95	LYS	N-CA-C	-5.14	105.37	111.69
2	B	118	ILE	CA-C-N	5.12	126.24	119.84
2	B	118	ILE	C-N-CA	5.12	126.24	119.84
2	B	84	ARG	N-CA-C	5.06	116.88	111.36
2	B	403	ILE	N-CA-C	-5.06	102.64	108.82
2	B	329	MET	N-CA-C	5.04	118.50	110.70
1	A	360	GLY	N-CA-C	-5.00	106.69	112.50

There are no chirality outliers.

There are no planarity outliers.

## 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	2665	0	2588	166	0
2	B	3154	0	3085	208	0
3	B	1	0	0	0	0
4	B	24	0	25	1	0
5	B	32	0	29	1	0
6	A	215	0	0	5	0
6	B	173	0	0	7	0
All	All	6264	0	5727	370	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 32.

All (370) 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)
2:B:282:MET:HG3	2:B:296:VAL:HG22	1.39	1.04
2:B:266:ARG:HH12	2:B:317:ALA:HB3	1.24	0.97
1:A:359:ILE:O	1:A:363:LEU:HD13	1.64	0.97
1:A:357:ARG:O	1:A:361:ARG:HD3	1.64	0.96
2:B:87:ARG:HG3	2:B:87:ARG:HH11	1.33	0.94
1:A:56:LEU:HD21	1:A:63:TYR:HA	1.51	0.93
2:B:151:ALA:HB3	2:B:152:PRO:HD3	1.53	0.90
2:B:285:GLU:HG2	2:B:296:VAL:HG21	1.54	0.90
1:A:342:GLU:OE1	1:A:346:LYS:HE3	1.71	0.90
2:B:66:HIS:HB3	2:B:67:LEU:HD13	1.54	0.89
2:B:189:GLY:O	2:B:225:THR:HG22	1.73	0.88
2:B:412:THR:O	2:B:416:LEU:HD13	1.76	0.86
1:A:294:ASN:O	1:A:298:GLN:HG2	1.76	0.85
2:B:124:THR:HG22	2:B:128:GLN:HE21	1.40	0.85
2:B:313:ARG:HG3	2:B:313:ARG:HH11	1.43	0.84
1:A:303:GLN:O	1:A:307:SER:HB2	1.77	0.82
2:B:331:HIS:CD2	2:B:334:ALA:H	1.98	0.80
2:B:389:VAL:HG22	2:B:391:GLU:OE1	1.82	0.80
2:B:67:LEU:HD13	2:B:67:LEU:H	1.43	0.80
1:A:80:GLN:HB2	1:A:104:ARG:NH2	1.97	0.79
2:B:266:ARG:NH1	2:B:317:ALA:HB3	1.97	0.79
2:B:131:GLU:HG2	2:B:171:VAL:HG13	1.65	0.78
2:B:308:LEU:HD12	2:B:330:PHE:CD2	2.18	0.78
1:A:351:ILE:HG23	1:A:352:ARG:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:VAL:O	1:A:320:GLU:HG3	1.83	0.77
1:A:106:VAL:HG13	1:A:111:GLU:HB3	1.67	0.77
1:A:108:GLN:HE21	1:A:108:GLN:CA	1.98	0.76
2:B:87:ARG:HG3	2:B:87:ARG:NH1	1.93	0.76
1:A:296:LEU:O	1:A:300:LEU:HD13	1.85	0.75
1:A:78:VAL:O	1:A:104:ARG:HD2	1.87	0.74
1:A:357:ARG:O	1:A:361:ARG:CD	2.36	0.73
2:B:301:SER:O	2:B:305:ALA:HB3	1.89	0.72
2:B:353:LYS:HB2	2:B:354:PRO:HD2	1.71	0.72
2:B:27:ARG:HG2	2:B:29:GLU:OE2	1.88	0.72
1:A:261:GLN:O	1:A:265:GLU:HG2	1.90	0.72
2:B:29:GLU:OE2	2:B:29:GLU:N	2.23	0.71
2:B:381:MET:C	2:B:382:LEU:HD22	2.16	0.71
1:A:56:LEU:HD22	1:A:63:TYR:HD1	1.56	0.70
2:B:178:LEU:HD21	2:B:182:TYR:CE1	2.25	0.70
1:A:263:THR:O	1:A:267:ILE:HG13	1.91	0.70
1:A:80:GLN:HB2	1:A:104:ARG:CZ	2.23	0.69
1:A:365:SER:OG	1:A:366:LYS:NZ	2.22	0.69
2:B:185:LYS:HD3	2:B:186:GLN:N	2.08	0.69
2:B:33:GLU:O	2:B:284:PHE:HB2	1.93	0.68
1:A:304:PRO:HG2	1:A:305:SER:H	1.60	0.67
2:B:26:LEU:HD13	2:B:59:PHE:HB3	1.77	0.67
2:B:285:GLU:CG	2:B:296:VAL:HG21	2.24	0.66
2:B:93:TYR:HD2	2:B:96:LEU:HD12	1.60	0.66
2:B:121:ILE:N	2:B:121:ILE:HD12	2.10	0.66
1:A:289:LEU:HD12	1:A:289:LEU:H	1.60	0.65
1:A:56:LEU:HD22	1:A:63:TYR:CD1	2.33	0.64
2:B:253:PHE:HA	2:B:307:LEU:HD21	1.81	0.63
2:B:331:HIS:HD2	2:B:334:ALA:H	1.46	0.63
1:A:108:GLN:HE21	1:A:108:GLN:HA	1.63	0.63
1:A:96:PHE:HA	1:A:126:LEU:HD13	1.78	0.63
2:B:91:ASP:O	2:B:94:GLU:HG3	1.98	0.63
1:A:94:GLU:HG3	1:A:97:ARG:NH1	2.14	0.62
1:A:302:LEU:HD22	1:A:306:HIS:HD2	1.63	0.62
2:B:78:HIS:O	2:B:82:LEU:HG	1.99	0.62
2:B:266:ARG:HH11	2:B:318:GLN:HG3	1.64	0.62
2:B:420:VAL:O	2:B:422:GLY:N	2.33	0.62
2:B:178:LEU:C	2:B:178:LEU:HD23	2.24	0.62
2:B:67:LEU:HD13	2:B:67:LEU:N	2.14	0.62
2:B:377:GLY:O	2:B:378:SER:HB2	1.98	0.61
2:B:64:PHE:O	2:B:66:HIS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD12	1:A:289:LEU:N	2.13	0.61
2:B:124:THR:CG2	2:B:128:GLN:HE21	2.13	0.61
2:B:158:ASN:O	2:B:162:ILE:HG13	2.00	0.61
1:A:302:LEU:HD22	1:A:306:HIS:CD2	2.35	0.61
2:B:31:ALA:O	2:B:34:ARG:HB2	2.00	0.61
2:B:412:THR:O	2:B:416:LEU:CD1	2.48	0.61
1:A:359:ILE:O	1:A:363:LEU:CD1	2.45	0.60
2:B:25:SER:OG	2:B:341:MET:HE1	2.01	0.60
1:A:138:ARG:HD2	1:A:174:VAL:HG11	1.83	0.60
2:B:93:TYR:CD2	2:B:96:LEU:HD12	2.36	0.60
2:B:266:ARG:N	2:B:266:ARG:HD2	2.17	0.60
2:B:23:LEU:HD11	2:B:71:LEU:HD11	1.83	0.60
2:B:328:TRP:H	2:B:332:GLN:NE2	2.00	0.60
1:A:223:VAL:HG11	1:A:240:ARG:HB2	1.82	0.59
1:A:319:TYR:HD2	1:A:322:MET:HE2	1.66	0.59
2:B:175:GLU:CD	2:B:175:GLU:H	2.10	0.59
2:B:337:GLU:HB3	2:B:341:MET:HE2	1.84	0.59
1:A:260:VAL:O	1:A:264:LEU:HG	2.03	0.58
2:B:34:ARG:HG2	2:B:34:ARG:HH11	1.68	0.58
2:B:23:LEU:CB	2:B:26:LEU:HD23	2.34	0.58
2:B:282:MET:HG3	2:B:296:VAL:CG2	2.25	0.58
1:A:255:VAL:HG13	1:A:258:ARG:NH2	2.18	0.58
2:B:173:ASN:ND2	2:B:176:LYS:HE2	2.19	0.58
1:A:327:CYS:SG	1:A:333:ILE:HD12	2.43	0.58
2:B:76:GLU:HG2	6:B:2108:HOH:O	2.04	0.58
2:B:89:LEU:HD11	2:B:103:LEU:HD13	1.85	0.58
2:B:178:LEU:HD13	2:B:421:PRO:HB2	1.85	0.58
2:B:302:PHE:CZ	2:B:402:ASN:HB2	2.39	0.58
2:B:350:LEU:N	2:B:350:LEU:HD22	2.19	0.57
1:A:264:LEU:O	1:A:268:LYS:HG3	2.03	0.57
2:B:265:GLU:CD	2:B:265:GLU:H	2.13	0.57
4:B:1001:FPP:H102	5:B:2001:736:H71	1.84	0.57
2:B:331:HIS:NE2	2:B:333:GLN:HB3	2.19	0.57
1:A:106:VAL:HG11	1:A:116:ALA:CB	2.35	0.57
2:B:266:ARG:HH12	2:B:317:ALA:CB	2.08	0.57
2:B:418:LYS:HD2	2:B:418:LYS:N	2.19	0.57
2:B:34:ARG:HE	2:B:52:GLU:HB3	1.69	0.57
2:B:29:GLU:O	2:B:32:ARG:HB2	2.04	0.57
2:B:174:ARG:HD2	2:B:415:PHE:HD2	1.69	0.57
2:B:337:GLU:HB3	2:B:341:MET:CE	2.35	0.57
1:A:312:ILE:CG2	1:A:344:LEU:HD21	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:CD2	1:A:63:TYR:HA	2.32	0.56
2:B:66:HIS:HB3	2:B:67:LEU:CD1	2.32	0.56
2:B:313:ARG:HH11	2:B:313:ARG:CG	2.16	0.56
1:A:104:ARG:O	1:A:108:GLN:HB2	2.06	0.56
1:A:108:GLN:CA	1:A:108:GLN:NE2	2.68	0.56
1:A:108:GLN:HA	1:A:108:GLN:NE2	2.20	0.56
2:B:127:CYS:O	2:B:131:GLU:HG3	2.06	0.56
1:A:58:LEU:HD21	1:A:122:ASP:HB3	1.86	0.56
1:A:156:THR:O	1:A:160:GLU:HG2	2.06	0.56
2:B:79:PHE:HD1	2:B:116:GLU:HG3	1.70	0.56
1:A:189:ILE:HG21	1:A:206:ARG:HB2	1.88	0.55
2:B:338:TYR:CE2	2:B:343:CYS:SG	2.99	0.55
2:B:118:ILE:HD12	2:B:118:ILE:N	2.21	0.55
2:B:297:ASP:HB3	2:B:300:TYR:CD1	2.42	0.55
1:A:84:PRO:C	1:A:86:PRO:HD3	2.31	0.55
1:A:231:VAL:CG2	1:A:266:MET:HE3	2.36	0.55
1:A:262:TYR:OH	1:A:266:MET:HE2	2.07	0.55
2:B:75:ARG:NH2	2:B:393:VAL:O	2.35	0.55
1:A:231:VAL:HG23	1:A:266:MET:HE3	1.88	0.55
2:B:335:LEU:HD23	2:B:373:ALA:HB2	1.88	0.55
2:B:398:HIS:ND1	2:B:399:PRO:HD2	2.22	0.55
2:B:151:ALA:HB3	2:B:152:PRO:CD	2.34	0.54
2:B:281:GLN:HB2	2:B:288:PHE:CE2	2.42	0.54
2:B:331:HIS:CD2	2:B:333:GLN:HB3	2.43	0.54
2:B:296:VAL:HG23	6:B:2002:HOH:O	2.07	0.54
1:A:106:VAL:HG11	1:A:116:ALA:HB1	1.89	0.54
1:A:148:LEU:HB2	1:A:179:LEU:HD21	1.88	0.54
2:B:308:LEU:HB2	2:B:309:PRO:HD3	1.90	0.54
2:B:398:HIS:CD2	2:B:408:VAL:HG21	2.43	0.54
2:B:62:TYR:C	2:B:64:PHE:H	2.16	0.54
2:B:166:GLU:O	2:B:170:ASN:OD1	2.26	0.53
1:A:170:HIS:O	1:A:174:VAL:HG23	2.08	0.53
1:A:319:TYR:CE1	1:A:336:LYS:HG2	2.44	0.53
1:A:289:LEU:H	1:A:289:LEU:CD1	2.20	0.53
2:B:27:ARG:HG2	2:B:29:GLU:CD	2.33	0.53
1:A:319:TYR:HA	1:A:322:MET:HE2	1.90	0.53
2:B:173:ASN:HD21	2:B:176:LYS:HE2	1.73	0.53
1:A:155:ILE:O	1:A:159:ILE:HG13	2.08	0.53
1:A:304:PRO:HG2	1:A:305:SER:N	2.23	0.53
2:B:174:ARG:HD2	2:B:415:PHE:CD2	2.44	0.53
2:B:296:VAL:HG12	2:B:297:ASP:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:N	1:A:300:LEU:HD12	2.24	0.52
2:B:135:SER:OG	2:B:136:PRO:HD2	2.08	0.52
1:A:239:GLN:O	1:A:243:VAL:HG23	2.09	0.52
2:B:310:LEU:HD21	2:B:400:VAL:HG22	1.90	0.52
1:A:135:HIS:O	1:A:139:VAL:HG23	2.10	0.52
1:A:365:SER:O	1:A:366:LYS:HE3	2.08	0.52
1:A:120:THR:O	1:A:124:ILE:HG13	2.08	0.52
1:A:354:GLU:OE2	2:B:327:HIS:HB2	2.10	0.52
2:B:280:ARG:HA	2:B:280:ARG:NE	2.25	0.52
1:A:94:GLU:HG3	1:A:97:ARG:HH12	1.75	0.52
1:A:329:ASN:HB3	1:A:332:ASP:HB3	1.91	0.52
2:B:82:LEU:HB2	2:B:111:LEU:HD21	1.92	0.52
2:B:134:GLN:HB2	2:B:140:PHE:CE2	2.44	0.51
1:A:151:GLU:HG3	1:A:175:LEU:HD11	1.92	0.51
1:A:233:ASN:CG	1:A:236:VAL:HG23	2.35	0.51
1:A:362:SER:C	1:A:364:GLN:H	2.17	0.51
1:A:362:SER:O	1:A:366:LYS:HD2	2.11	0.51
2:B:89:LEU:CD1	2:B:103:LEU:HD13	2.40	0.51
1:A:65:LEU:HD11	6:A:581:HOH:O	2.11	0.51
1:A:322:MET:HB3	1:A:327:CYS:SG	2.51	0.51
2:B:90:THR:C	2:B:92:ALA:H	2.18	0.51
1:A:167:GLN:CD	1:A:167:GLN:H	2.19	0.50
1:A:165:ASN:HB3	1:A:168:VAL:HG22	1.94	0.50
1:A:319:TYR:O	1:A:323:LEU:HD13	2.11	0.50
1:A:117:PHE:CE2	1:A:146:LYS:HE2	2.47	0.50
1:A:287:ARG:HG2	1:A:291:ARG:HD2	1.93	0.50
1:A:364:GLN:HA	1:A:364:GLN:NE2	2.26	0.50
2:B:98:ALA:O	2:B:142:GLY:HA3	2.12	0.50
1:A:182:PRO:HG3	1:A:213:PHE:CD2	2.47	0.50
1:A:220:LEU:HB2	1:A:243:VAL:HG11	1.94	0.50
2:B:265:GLU:HG2	2:B:314:ALA:HB2	1.94	0.50
2:B:326:SER:HB2	2:B:383:HIS:ND1	2.27	0.50
2:B:260:VAL:HA	2:B:265:GLU:OE2	2.11	0.49
1:A:296:LEU:O	1:A:300:LEU:CD1	2.57	0.49
1:A:357:ARG:O	1:A:361:ARG:CG	2.60	0.49
2:B:27:ARG:O	2:B:30:HIS:HB3	2.13	0.49
2:B:84:ARG:O	2:B:85:GLY:C	2.55	0.49
2:B:124:THR:HG22	2:B:128:GLN:NE2	2.19	0.49
1:A:312:ILE:HG21	1:A:344:LEU:HD21	1.94	0.49
1:A:319:TYR:HE1	1:A:336:LYS:HG2	1.76	0.49
2:B:119:PRO:HB2	2:B:122:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:VAL:O	1:A:247:THR:HG23	2.13	0.49
1:A:56:LEU:CD2	1:A:63:TYR:HD1	2.25	0.49
1:A:87:VAL:O	1:A:88:VAL:C	2.56	0.49
1:A:351:ILE:O	2:B:331:HIS:HB2	2.13	0.49
2:B:74:GLN:HA	2:B:74:GLN:NE2	2.28	0.49
2:B:71:LEU:N	2:B:71:LEU:HD12	2.27	0.49
2:B:239:ILE:HB	2:B:252:THR:HA	1.94	0.49
2:B:194:HIS:HB2	6:B:2021:HOH:O	2.12	0.49
2:B:73:LEU:HD12	2:B:344:GLN:OE1	2.13	0.48
2:B:121:ILE:N	2:B:121:ILE:CD1	2.76	0.48
1:A:135:HIS:CD2	2:B:147:TYR:HE1	2.32	0.48
1:A:301:ASP:O	1:A:304:PRO:HD2	2.14	0.48
2:B:69:PRO:HG2	6:B:2074:HOH:O	2.13	0.48
2:B:178:LEU:HD11	2:B:218:THR:HG23	1.96	0.48
1:A:319:TYR:HD2	1:A:322:MET:CE	2.25	0.48
1:A:328:ASP:O	1:A:329:ASN:HB2	2.14	0.48
1:A:361:ARG:NH1	2:B:322:ALA:O	2.47	0.48
2:B:23:LEU:HB3	2:B:26:LEU:HD23	1.94	0.48
2:B:412:THR:C	2:B:416:LEU:HD13	2.39	0.48
1:A:360:GLY:O	1:A:364:GLN:HB2	2.13	0.48
2:B:64:PHE:O	2:B:66:HIS:ND1	2.42	0.48
2:B:117:PRO:O	2:B:119:PRO:HD3	2.14	0.48
1:A:193:LEU:HD21	1:A:202:ALA:HB3	1.95	0.47
2:B:308:LEU:CD1	2:B:330:PHE:HD2	2.28	0.47
1:A:74:ASP:OD1	1:A:75:ILE:HG13	2.13	0.47
1:A:265:GLU:O	1:A:269:LEU:HD23	2.14	0.47
1:A:287:ARG:HD3	1:A:292:TYR:OH	2.15	0.47
1:A:239:GLN:HA	1:A:239:GLN:OE1	2.14	0.47
1:A:103:PHE:HE1	1:A:120:THR:HG22	1.80	0.47
1:A:275:SER:OG	2:B:293:ASN:ND2	2.48	0.47
1:A:295:LEU:O	1:A:296:LEU:C	2.58	0.47
1:A:302:LEU:CD2	1:A:306:HIS:HD2	2.27	0.47
2:B:308:LEU:CD1	2:B:330:PHE:CD2	2.93	0.47
2:B:134:GLN:HE22	2:B:173:ASN:H	1.62	0.47
1:A:185:GLU:O	1:A:189:ILE:HG13	2.15	0.47
2:B:404:GLY:O	2:B:408:VAL:HG23	2.15	0.47
2:B:304:GLN:OE1	2:B:304:GLN:HA	2.15	0.46
2:B:308:LEU:HD23	2:B:308:LEU:HA	1.53	0.46
2:B:90:THR:C	2:B:92:ALA:N	2.73	0.46
2:B:135:SER:C	2:B:137:ASP:H	2.23	0.46
1:A:96:PHE:C	1:A:96:PHE:CD2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:C	1:A:56:LEU:HD23	2.40	0.46
1:A:58:LEU:O	1:A:95:LYS:NZ	2.47	0.46
2:B:117:PRO:C	2:B:118:ILE:HD12	2.41	0.46
2:B:277:VAL:O	2:B:280:ARG:HB2	2.15	0.46
2:B:75:ARG:NE	2:B:391:GLU:O	2.46	0.46
1:A:223:VAL:HG13	1:A:236:VAL:CG1	2.46	0.46
1:A:66:TYR:CE2	1:A:119:LEU:HD13	2.50	0.46
1:A:336:LYS:O	1:A:340:LEU:HG	2.16	0.46
1:A:344:LEU:HD13	1:A:356:TRP:CE2	2.51	0.46
2:B:66:HIS:CB	2:B:67:LEU:HD13	2.37	0.46
2:B:211:ALA:HA	2:B:216:ILE:HG12	1.98	0.46
2:B:353:LYS:HB2	2:B:354:PRO:CD	2.45	0.46
1:A:294:ASN:C	1:A:298:GLN:HG2	2.38	0.45
2:B:281:GLN:HB2	2:B:288:PHE:CZ	2.52	0.45
2:B:310:LEU:CD2	2:B:400:VAL:HG22	2.46	0.45
1:A:328:ASP:O	1:A:329:ASN:CB	2.63	0.45
2:B:26:LEU:N	2:B:26:LEU:HD22	2.31	0.45
2:B:119:PRO:O	2:B:122:VAL:HG12	2.15	0.45
2:B:87:ARG:NH1	2:B:87:ARG:CG	2.69	0.45
1:A:303:GLN:OE1	1:A:303:GLN:HA	2.16	0.45
1:A:300:LEU:CD1	1:A:300:LEU:H	2.30	0.45
1:A:173:ARG:O	1:A:177:GLU:HG3	2.16	0.45
1:A:231:VAL:O	1:A:231:VAL:HG22	2.15	0.45
1:A:326:GLN:CD	1:A:326:GLN:N	2.74	0.45
2:B:370:LEU:HD23	2:B:394:LEU:HD11	1.98	0.45
2:B:96:LEU:HD13	2:B:103:LEU:HD21	1.99	0.45
2:B:351:LEU:C	2:B:351:LEU:HD12	2.42	0.45
2:B:130:LEU:HD12	2:B:160:LEU:HD21	1.99	0.45
2:B:266:ARG:HD2	2:B:266:ARG:H	1.81	0.45
2:B:313:ARG:CG	2:B:313:ARG:NH1	2.79	0.45
2:B:75:ARG:NH2	2:B:391:GLU:O	2.49	0.44
1:A:268:LYS:O	1:A:271:PRO:HD3	2.17	0.44
2:B:23:LEU:CD1	2:B:71:LEU:HD11	2.45	0.44
2:B:71:LEU:HB3	2:B:340:LEU:HD13	1.98	0.44
2:B:178:LEU:HD23	2:B:178:LEU:O	2.17	0.44
2:B:389:VAL:CG2	2:B:391:GLU:OE1	2.60	0.44
1:A:287:ARG:HE	1:A:291:ARG:CD	2.30	0.44
1:A:320:GLU:O	1:A:324:GLU:HG3	2.17	0.44
1:A:336:LYS:HB2	1:A:336:LYS:HE3	1.70	0.44
1:A:362:SER:C	1:A:364:GLN:N	2.75	0.44
2:B:266:ARG:HE	2:B:318:GLN:NE2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:HA	6:A:496:HOH:O	2.17	0.44
2:B:84:ARG:O	2:B:87:ARG:N	2.43	0.44
2:B:151:ALA:CB	2:B:152:PRO:HD3	2.37	0.44
2:B:389:VAL:CG2	2:B:390:PRO:HD2	2.48	0.44
1:A:56:LEU:HD21	1:A:63:TYR:CA	2.33	0.44
2:B:232:CYS:CB	2:B:239:ILE:HG23	2.47	0.44
1:A:342:GLU:OE2	1:A:342:GLU:HA	2.18	0.44
2:B:232:CYS:HB2	2:B:239:ILE:HG23	2.00	0.44
2:B:359:ASP:CG	2:B:362:HIS:HD1	2.25	0.44
2:B:381:MET:O	2:B:382:LEU:HD22	2.17	0.44
1:A:85:SER:N	1:A:86:PRO:HD3	2.33	0.43
2:B:23:LEU:HB2	2:B:26:LEU:HD23	1.99	0.43
2:B:34:ARG:HG2	2:B:34:ARG:NH1	2.32	0.43
2:B:73:LEU:O	2:B:75:ARG:N	2.42	0.43
1:A:319:TYR:HA	1:A:322:MET:CE	2.48	0.43
1:A:219:GLU:O	1:A:223:VAL:HG23	2.18	0.43
1:A:296:LEU:CD1	1:A:300:LEU:HD11	2.47	0.43
1:A:300:LEU:HD12	1:A:300:LEU:H	1.83	0.43
2:B:178:LEU:C	2:B:178:LEU:CD2	2.89	0.43
1:A:92:TYR:C	1:A:93:SER:O	2.57	0.43
1:A:223:VAL:HG13	1:A:236:VAL:HG12	2.00	0.43
2:B:405:PRO:O	2:B:409:ILE:HG13	2.17	0.43
2:B:412:THR:HG21	6:B:2173:HOH:O	2.18	0.43
1:A:219:GLU:OE1	1:A:219:GLU:HA	2.18	0.43
2:B:350:LEU:HD23	2:B:363:THR:HG23	2.01	0.43
2:B:383:HIS:C	2:B:383:HIS:CD2	2.97	0.43
1:A:66:TYR:CZ	1:A:119:LEU:HD13	2.53	0.43
1:A:205:HIS:O	1:A:209:VAL:HG23	2.18	0.43
1:A:136:PHE:CE2	1:A:140:LEU:HD11	2.54	0.43
2:B:284:PHE:HB3	2:B:285:GLU:OE2	2.18	0.43
1:A:144:LEU:O	1:A:145:GLN:C	2.62	0.43
2:B:29:GLU:HA	2:B:32:ARG:HD3	2.00	0.43
2:B:333:GLN:HG3	2:B:387:MET:HE2	2.00	0.43
2:B:389:VAL:HG13	2:B:392:ASN:ND2	2.34	0.43
1:A:71:GLU:HG2	1:A:72:TRP:CD1	2.54	0.42
2:B:285:GLU:CD	2:B:285:GLU:H	2.28	0.42
2:B:351:LEU:HD22	2:B:356:LYS:O	2.20	0.42
1:A:289:LEU:N	1:A:289:LEU:CD1	2.80	0.42
1:A:353:LYS:O	1:A:357:ARG:HB2	2.20	0.42
2:B:82:LEU:CB	2:B:111:LEU:HD21	2.48	0.42
2:B:178:LEU:HB2	2:B:216:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:HIS:HB3	2:B:332:GLN:NE2	2.34	0.42
2:B:327:HIS:HB3	2:B:332:GLN:HE21	1.84	0.42
1:A:287:ARG:HE	1:A:291:ARG:HH21	1.66	0.42
1:A:299:LEU:HB3	1:A:311:LEU:HD11	2.01	0.42
1:A:109:ARG:O	1:A:110:ASP:C	2.62	0.42
1:A:319:TYR:O	1:A:323:LEU:CD1	2.67	0.42
2:B:86:LEU:CD2	2:B:122:VAL:HG21	2.49	0.42
2:B:274:LEU:O	2:B:278:THR:HG23	2.19	0.42
2:B:411:ALA:HB2	6:B:2105:HOH:O	2.18	0.42
1:A:300:LEU:HA	1:A:303:GLN:HG2	2.02	0.42
2:B:351:LEU:HD13	2:B:353:LYS:O	2.20	0.42
1:A:355:TYR:O	1:A:358:TYR:HB3	2.19	0.42
1:A:322:MET:HB3	1:A:327:CYS:HB3	2.01	0.42
2:B:48:GLN:HA	2:B:48:GLN:NE2	2.34	0.42
1:A:256:LEU:O	1:A:260:VAL:HG23	2.20	0.42
1:A:319:TYR:CD2	1:A:322:MET:CE	3.03	0.41
2:B:350:LEU:N	2:B:350:LEU:CD2	2.83	0.41
1:A:289:LEU:HD23	1:A:314:PHE:CE2	2.55	0.41
1:A:323:LEU:HD21	1:A:334:LEU:HD13	2.00	0.41
1:A:213:PHE:CD1	1:A:213:PHE:N	2.88	0.41
2:B:216:ILE:HA	2:B:420:VAL:HG13	2.02	0.41
2:B:67:LEU:H	2:B:67:LEU:CD1	2.25	0.41
2:B:109:HIS:O	2:B:112:GLU:HB3	2.21	0.41
2:B:333:GLN:HE21	2:B:387:MET:HE1	1.85	0.41
2:B:38:ASP:O	2:B:40:VAL:HG23	2.20	0.41
2:B:285:GLU:HG2	2:B:296:VAL:CG2	2.38	0.41
2:B:221:LEU:HD23	2:B:222:PHE:CE1	2.56	0.41
1:A:79:PRO:HA	1:A:101:ASP:OD1	2.20	0.41
2:B:74:GLN:HA	2:B:74:GLN:HE21	1.85	0.41
1:A:138:ARG:HH11	1:A:138:ARG:HD3	1.70	0.41
1:A:138:ARG:HG3	1:A:178:TRP:CH2	2.55	0.41
1:A:263:THR:HG21	1:A:280:LEU:HB2	2.02	0.41
1:A:366:LYS:HD2	1:A:366:LYS:N	2.35	0.41
2:B:73:LEU:H	2:B:392:ASN:ND2	2.18	0.41
2:B:294:LYS:HA	2:B:294:LYS:HD2	1.79	0.41
2:B:398:HIS:HD2	2:B:408:VAL:HG21	1.82	0.41
1:A:322:MET:HE3	1:A:333:ILE:HG21	2.02	0.41
2:B:266:ARG:H	2:B:266:ARG:CD	2.35	0.41
2:B:333:GLN:HG3	2:B:387:MET:CE	2.51	0.41
1:A:125:GLU:HB2	6:A:404:HOH:O	2.20	0.40
1:A:242:PHE:HA	6:A:372:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:N	1:A:300:LEU:CD1	2.84	0.40
2:B:377:GLY:O	2:B:378:SER:CB	2.64	0.40
1:A:287:ARG:NH1	6:A:478:HOH:O	2.54	0.40
1:A:333:ILE:O	1:A:336:LYS:HB3	2.21	0.40
2:B:67:LEU:N	2:B:67:LEU:CD1	2.82	0.40
2:B:86:LEU:HD21	2:B:122:VAL:HG21	2.03	0.40
2:B:225:THR:O	2:B:229:ILE:HG13	2.21	0.40
2:B:266:ARG:N	2:B:266:ARG:CD	2.82	0.40
2:B:280:ARG:O	2:B:289:GLN:HG2	2.21	0.40
2:B:417:GLN:HB2	2:B:418:LYS:HD2	2.03	0.40
1:A:308:SER:HB2	1:A:309:PRO:HD2	2.04	0.40
2:B:217:ILE:HB	6:B:2087:HOH:O	2.22	0.40
2:B:274:LEU:HD21	2:B:329:MET:HE1	2.04	0.40
1:A:80:GLN:HB2	1:A:104:ARG:HH21	1.81	0.40
1:A:296:LEU:O	1:A:297:ASN:C	2.64	0.40
2:B:29:GLU:HB3	2:B:32:ARG:NH1	2.37	0.40
2:B:327:HIS:HA	2:B:332:GLN:HE22	1.85	0.40
2:B:363:THR:O	2:B:367:LEU:HG	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	311/313 (99%)	273 (88%)	32 (10%)	6 (2%)	<b>6</b>   <b>17</b>
2	B	399/401 (100%)	359 (90%)	32 (8%)	8 (2%)	<b>6</b>   <b>16</b>
All	All	710/714 (99%)	632 (89%)	64 (9%)	14 (2%)	<b>6</b>   <b>16</b>

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ASP
1	A	287	ARG
1	A	329	ASN
2	B	65	ASN
2	B	378	SER
2	B	421	PRO
2	B	74	GLN
2	B	352	ASP
1	A	128	ALA
1	A	304	PRO
2	B	119	PRO
1	A	182	PRO
2	B	28	PRO
2	B	164	GLY

### 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	291/291 (100%)	277 (95%)	14 (5%)	23 50
2	B	338/338 (100%)	302 (89%)	36 (11%)	6 16
All	All	629/629 (100%)	579 (92%)	50 (8%)	11 28

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	61	PRO
1	A	77	PRO
1	A	79	PRO
1	A	84	PRO
1	A	86	PRO
1	A	108	GLN
1	A	163	PRO
1	A	182	PRO
1	A	271	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	293	PRO
1	A	304	PRO
1	A	309	PRO
1	A	366	LYS
2	B	26	LEU
2	B	28	PRO
2	B	29	GLU
2	B	67	LEU
2	B	69	PRO
2	B	87	ARG
2	B	101	PRO
2	B	117	PRO
2	B	118	ILE
2	B	119	PRO
2	B	121	ILE
2	B	136	PRO
2	B	144	PRO
2	B	148	PRO
2	B	152	PRO
2	B	175	GLU
2	B	178	LEU
2	B	185	LYS
2	B	187	PRO
2	B	219	PRO
2	B	243	PRO
2	B	265	GLU
2	B	285	GLU
2	B	309	PRO
2	B	313	ARG
2	B	321	PRO
2	B	346	PRO
2	B	350	LEU
2	B	354	PRO
2	B	390	PRO
2	B	396	PRO
2	B	399	PRO
2	B	405	PRO
2	B	418	LYS
2	B	419	PRO
2	B	421	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	135	HIS
1	A	184	GLN
1	A	204	GLN
1	A	241	HIS
1	A	246	ASN
1	A	285	GLN
1	A	294	ASN
1	A	306	HIS
1	A	325	ASN
1	A	364	GLN
2	B	48	GLN
2	B	56	GLN
2	B	74	GLN
2	B	88	GLN
2	B	128	GLN
2	B	134	GLN
2	B	179	GLN
2	B	275	GLN
2	B	293	ASN
2	B	318	GLN
2	B	327	HIS
2	B	331	HIS
2	B	332	GLN
2	B	336	GLN
2	B	392	ASN
2	B	410	GLN
2	B	417	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

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FPP	B	1001	-	22,23,23	0.75	1 (4%)	27,31,31	1.10	3 (11%)
5	736	B	2001	-	36,36,36	1.96	11 (30%)	40,53,53	1.28	6 (15%)

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
4	FPP	B	1001	-	-	8/25/25/25	-
5	736	B	2001	-	-	2/10/48/48	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	2001	736	S1-N27	6.26	1.73	1.63
5	B	2001	736	C11-C10	4.41	1.45	1.40
5	B	2001	736	C12-N1	3.58	1.48	1.37
5	B	2001	736	C18-C10	2.83	1.43	1.39
5	B	2001	736	C21-C20	2.72	1.42	1.38
5	B	2001	736	C19-C20	2.61	1.42	1.38
5	B	2001	736	C4-C13	2.57	1.50	1.46
5	B	2001	736	C19-C18	2.43	1.42	1.38
5	B	2001	736	C13-C12	2.41	1.38	1.35
5	B	2001	736	C21-C11	2.25	1.43	1.39
4	B	1001	FPP	PA-O3A	-2.15	1.57	1.59
5	B	2001	736	C6-C5	2.04	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2001	736	O2-S1-N27	-3.05	104.47	107.02
5	B	2001	736	O1-S1-N27	-2.92	104.58	107.02
5	B	2001	736	C1-N2-C3	2.80	122.50	116.92
4	B	1001	FPP	C6-C7-C8	-2.44	122.03	127.62
4	B	1001	FPP	C10-C8-C9	2.17	118.99	115.23
4	B	1001	FPP	C15-C13-C14	2.15	119.53	114.59
5	B	2001	736	C26-N27-S1	2.13	120.13	116.71
5	B	2001	736	C28-N27-S1	2.09	120.07	116.71
5	B	2001	736	C6-C1-N2	-2.06	120.16	123.42

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1001	FPP	C6-C7-C8-C10
4	B	1001	FPP	C6-C7-C8-C9
5	B	2001	736	C28-N27-S1-O2
5	B	2001	736	C28-N27-S1-C15
4	B	1001	FPP	C1-C2-C3-C4
4	B	1001	FPP	C1-C2-C3-C5
4	B	1001	FPP	PB-O3A-PA-O2A
4	B	1001	FPP	C4-C3-C5-C6
4	B	1001	FPP	C2-C3-C5-C6
4	B	1001	FPP	PB-O3A-PA-O1A

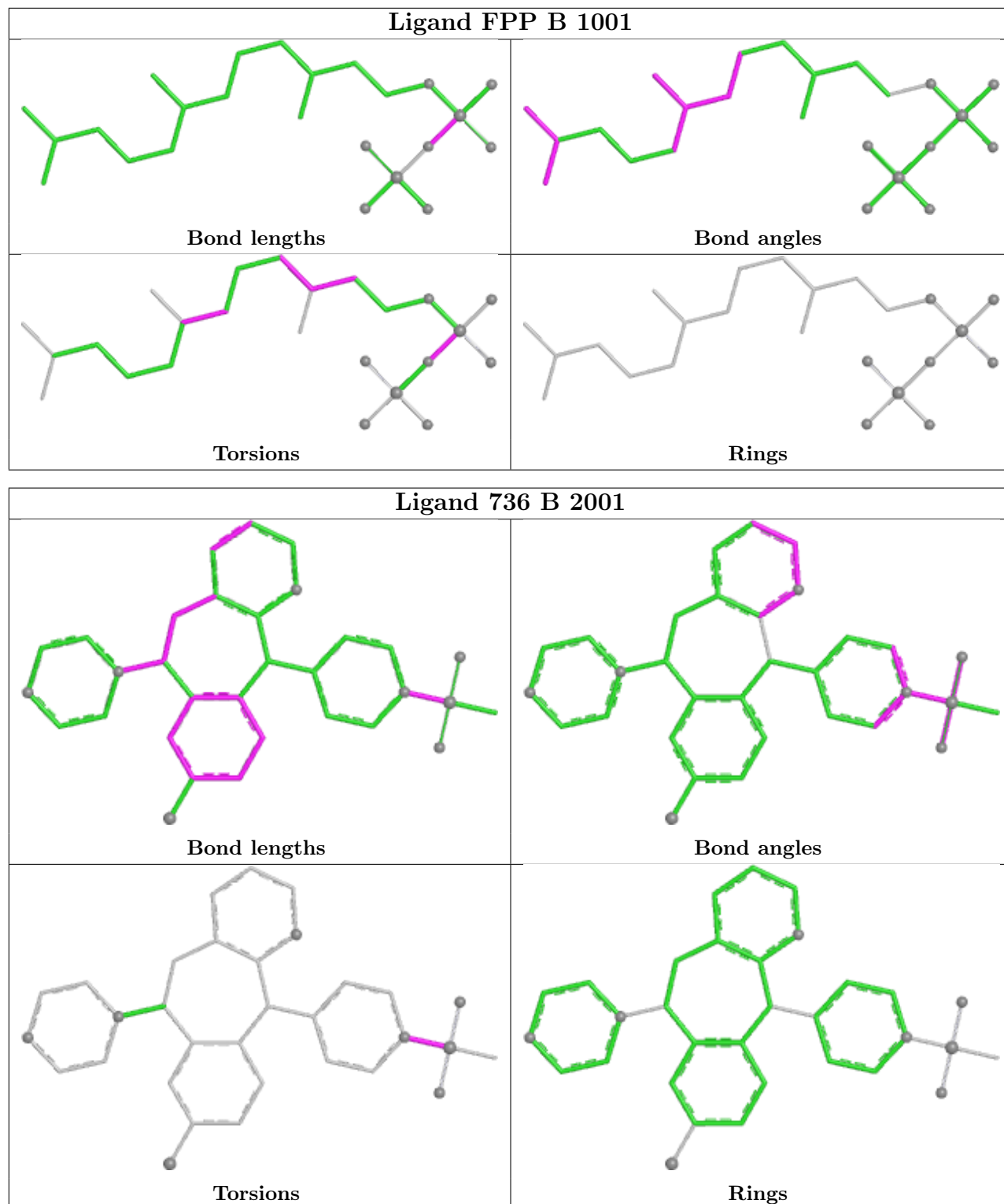
There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1001	FPP	1	0
5	B	2001	736	1	0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	313/313 (100%)	0.05	8 (2%) 57 54	26, 53, 94, 111	0
2	B	401/401 (100%)	0.09	11 (2%) 56 53	24, 51, 80, 110	0
All	All	714/714 (100%)	0.07	19 (2%) 56 53	24, 52, 85, 111	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	423	PHE	4.6
2	B	67	LEU	4.1
1	A	54	GLY	3.5
2	B	64	PHE	3.1
2	B	65	ASN	3.0
2	B	66	HIS	2.7
2	B	422	GLY	2.6
1	A	361	ARG	2.6
2	B	68	VAL	2.5
2	B	118	ILE	2.4
1	A	55	PHE	2.4
1	A	320	GLU	2.3
2	B	377	GLY	2.3
1	A	330	LYS	2.2
1	A	363	LEU	2.1
1	A	365	SER	2.1
2	B	283	ARG	2.1
1	A	357	ARG	2.1
2	B	87	ARG	2.0

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

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

### 6.3 Carbohydrates

There are no oligosaccharides in this entry.

### 6.4 Ligands

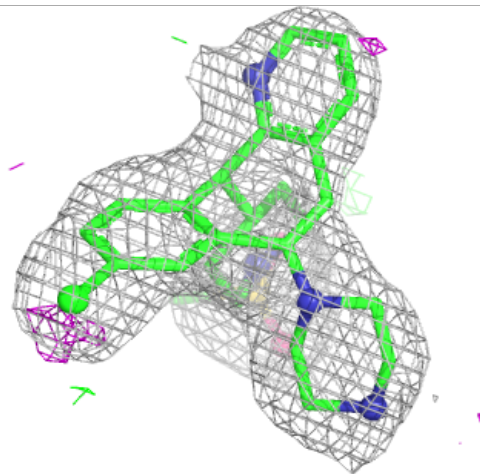
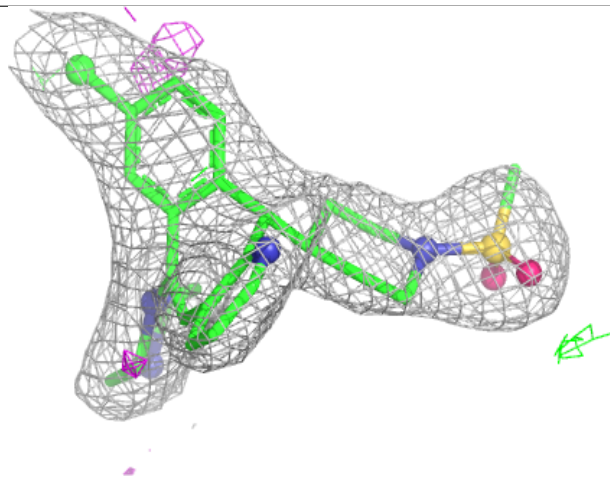
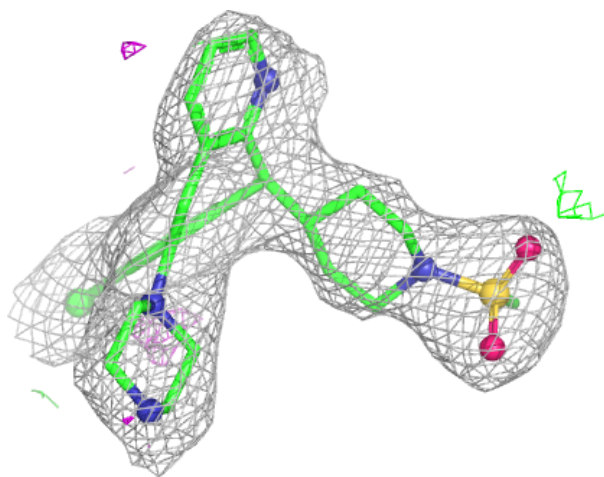
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

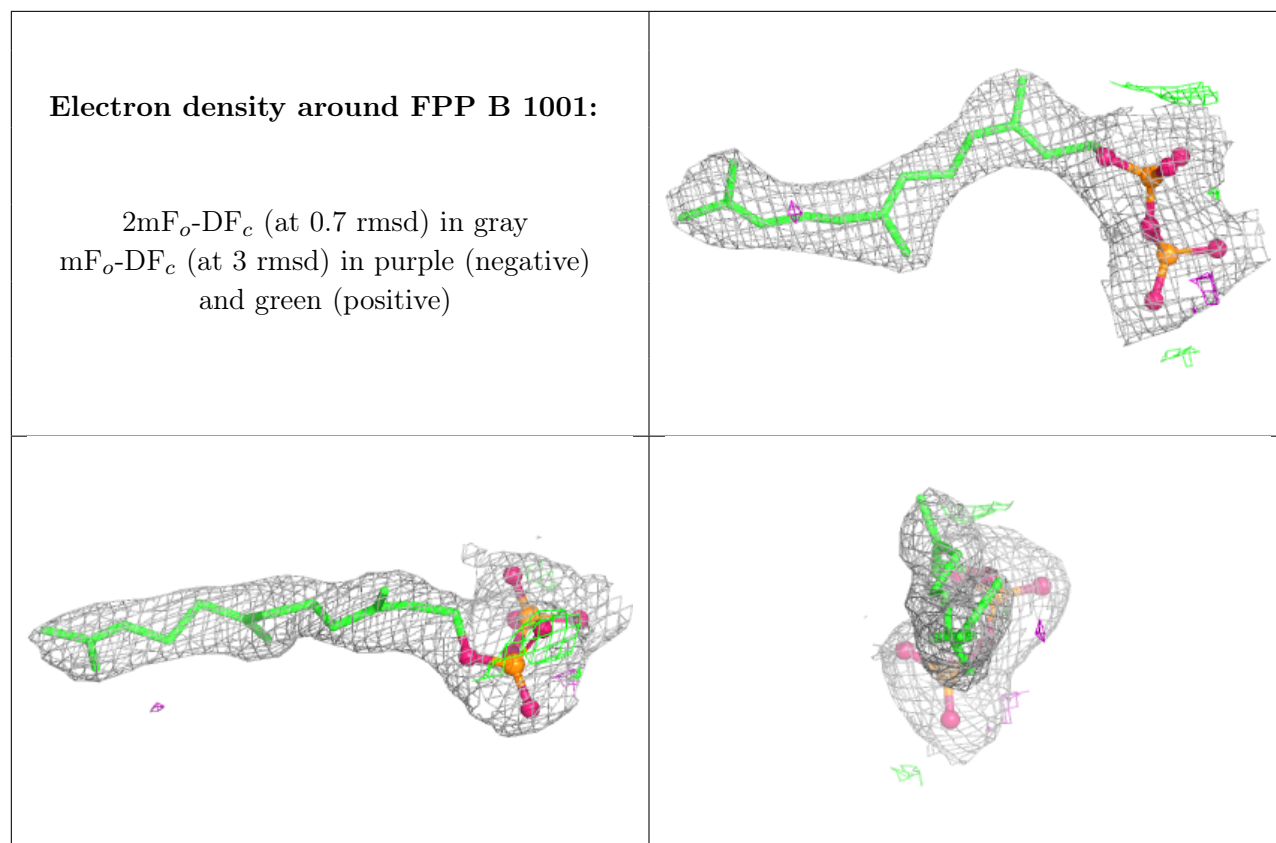
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	736	B	2001	32/32	0.95	0.09	39,52,58,59	0
4	FPP	B	1001	24/24	0.98	0.07	15,36,41,43	0
3	ZN	B	1	1/1	0.98	0.04	66,66,66,66	0

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 736 B 2001:**

$2mF_o-DF_c$  (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.