



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:27 pm BST

PDB ID : 1FDJ
Title : FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM RABBIT LIVER
Authors : Blom, N.S.; White, A.; Sygusch, J.
Deposited on : 2000-07-20
Resolution : 2.10 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)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

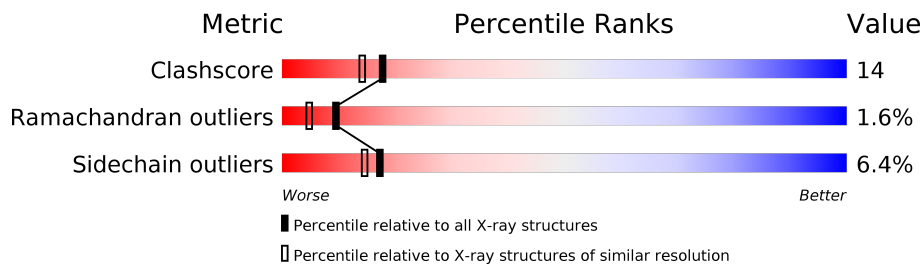
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	

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	2FP	A	5001	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2FP	B	6001	X	-	-	-
4	13P	C	7001	-	-	X	-
4	13P	D	8002[A]	-	-	X	-
5	G3P	B	6003	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15089 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 FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2820	1766	506	535	13	0	6	0
1	B	363	2918	1834	517	554	13	0	18	0
1	C	363	2914	1827	524	550	13	0	17	0
1	D	363	2850	1787	506	544	13	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

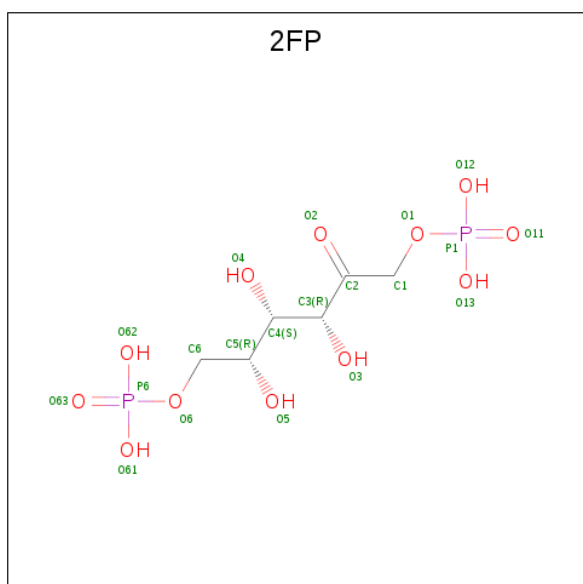
Chain	Residue	Modelled	Actual	Comment	Reference
A	1051	SER	THR	CONFLICT	UNP P79226
B	2051	SER	THR	CONFLICT	UNP P79226
C	3051	SER	THR	CONFLICT	UNP P79226
D	4051	SER	THR	CONFLICT	UNP P79226

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



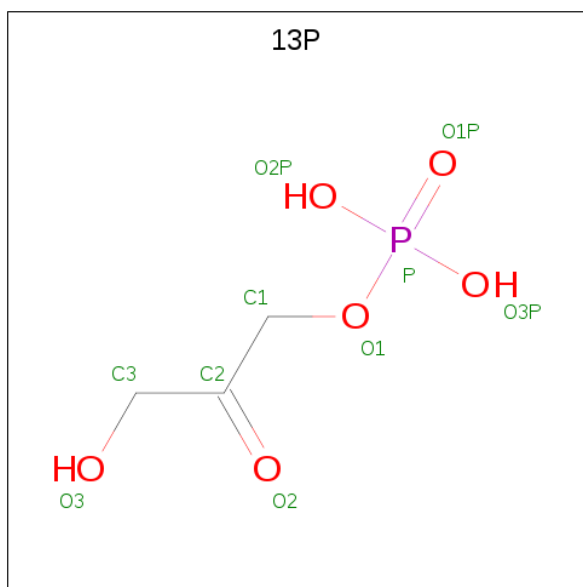
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,6-FRUCTOSE DIPHOSPHATE (LINEAR FORM) (three-letter code: 2FP) (formula: $C_6H_{14}O_{12}P_2$).



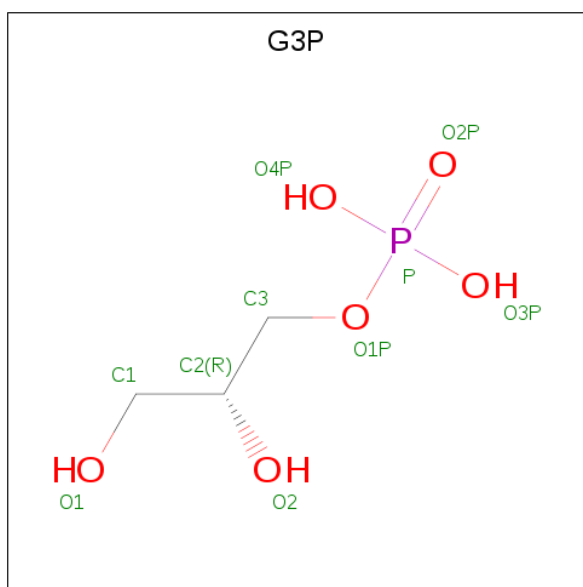
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			10	3	6	1		
4	C	1	Total	C	O	P	0	0
			10	3	6	1		
4	D	1	Total	C	O	P	0	1
			10	3	6	1		
4	D	1	Total	C	O	P	0	1
			10	3	6	1		

- Molecule 5 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
5	B	1	10	3	6	1	0	0

- Molecule 6 is water.

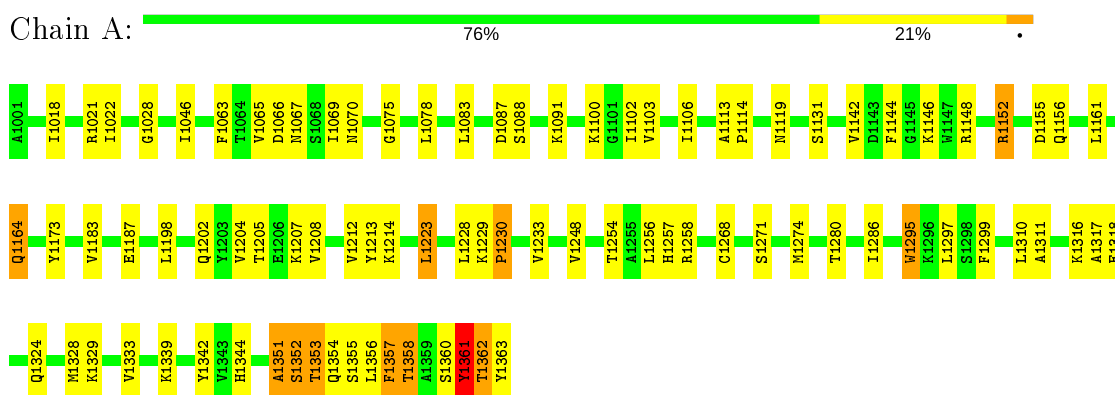
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	775	Total	O	0	0
			775	775		
6	B	858	Total	O	0	0
			858	858		
6	C	917	Total	O	0	0
			917	917		
6	D	927	Total	O	0	0
			927	927		

3 Residue-property plots

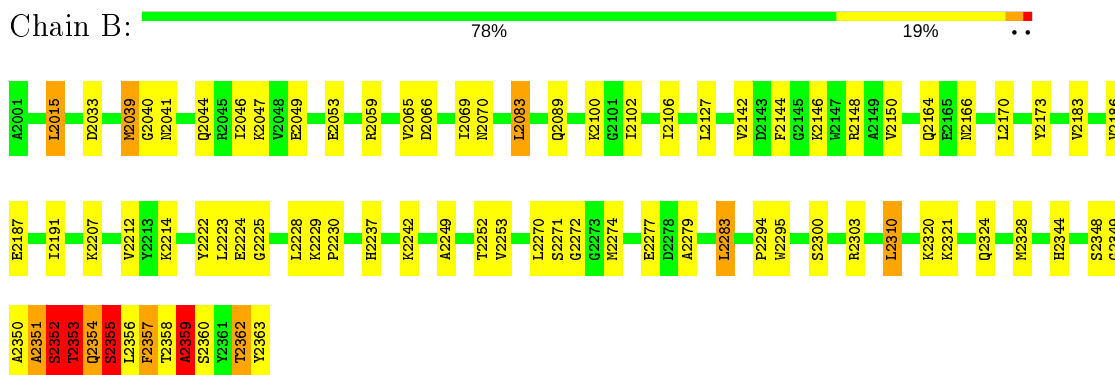
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

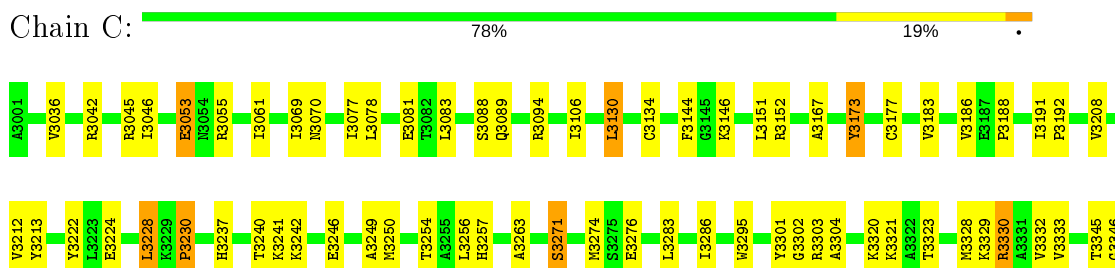
- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE



- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE



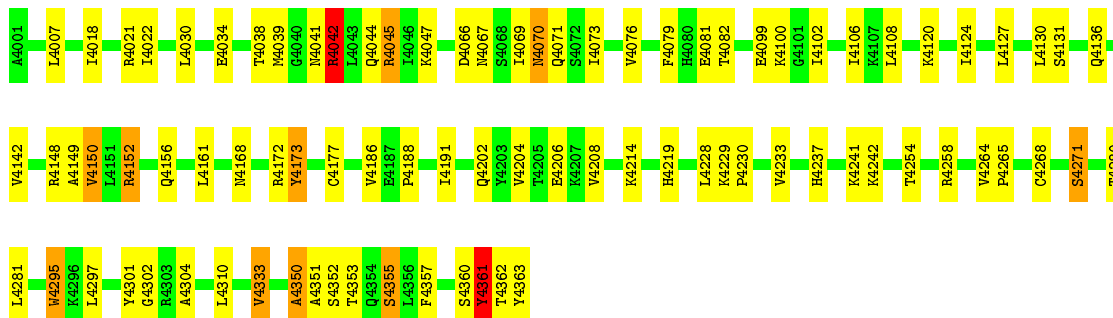
- Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE





● Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain D: 76% 20%



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	377.25Å 130.54Å 80.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.10	Depositor
% Data completeness (in resolution range)	8.0 (12.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.171 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15089	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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: G3P, 2FP, SO4, 13P

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	0.35	0/2869	0.64	0/3880
1	B	0.44	1/2973 (0.0%)	0.73	7/4023 (0.2%)
1	C	0.33	0/2966	0.62	0/4010
1	D	0.41	0/2900	0.69	2/3922 (0.1%)
All	All	0.38	1/11708 (0.0%)	0.67	9/15835 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2352	SER	N-CA	-6.02	1.34	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2353	THR	N-CA-C	7.00	129.89	111.00
1	B	2352	SER	CA-C-N	-6.77	102.30	117.20
1	B	2354	GLN	N-CA-C	-6.73	92.84	111.00
1	B	2353	THR	CA-C-N	-6.60	102.68	117.20
1	D	4042[A]	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	D	4042[B]	ARG	NE-CZ-NH2	6.33	123.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2039	MET	CG-SD-CE	6.30	110.28	100.20
1	B	2351	ALA	CA-C-N	-5.36	105.40	117.20
1	B	2359	ALA	CA-C-N	-5.26	105.62	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1213	TYR	Sidechain
1	B	2353	THR	Mainchain

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	2820	0	2831	60	0
1	B	2918	0	2912	89	0
1	C	2914	0	2928	68	0
1	D	2850	0	2853	92	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	0	10	2	0
3	B	20	0	8	5	0
4	B	10	0	1	1	0
4	C	10	0	5	6	0
4	D	20	0	10	7	0
5	B	10	0	4	3	0
6	A	775	0	0	12	0
6	B	858	0	0	33	0
6	C	917	0	0	24	0
6	D	927	0	0	32	0
All	All	15089	0	11562	315	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 14.

All (315) 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:D:4363[B]:TYR:CD2	6:D:8916:HOH:O	1.72	1.28
1:D:4042[A]:ARG:HG3	1:D:4042[A]:ARG:HH11	0.97	1.10
1:D:4363[B]:TYR:OH	6:D:8918:HOH:O	1.74	1.04
1:D:4042[A]:ARG:HG3	1:D:4042[A]:ARG:NH1	1.74	0.98
1:D:4363[B]:TYR:CE1	6:D:8917:HOH:O	2.16	0.98
4:C:7001:13P:H11	6:C:7892:HOH:O	1.66	0.96
4:C:7001:13P:O3	6:C:7890:HOH:O	1.82	0.95
1:D:4363[A]:TYR:HB3	6:D:8916:HOH:O	1.66	0.95
1:B:2354:GLN:HB3	6:B:6249:HOH:O	1.65	0.93
5:B:6003:G3P:O1	6:B:6781:HOH:O	1.89	0.91
1:B:2053:GLU:HG3	1:C:3053:GLU:HG3	1.51	0.91
1:C:3077:ILE:HD13	1:C:3146[B]:LYS:HD2	1.54	0.90
1:B:2146[A]:LYS:HG3	6:B:6801:HOH:O	1.72	0.88
1:D:4363[A]:TYR:HD2	6:D:8924:HOH:O	1.57	0.86
1:D:4237:HIS:HB3	1:D:4357:PHE:CD1	2.12	0.84
1:D:4042[A]:ARG:NH2	6:D:8922:HOH:O	2.11	0.83
1:B:2148:ARG:HD3	5:B:6003:G3P:H12	1.63	0.80
1:D:4073:ILE:HG21	6:D:8492:HOH:O	1.82	0.80
1:D:4150:VAL:HB	1:D:4361[A]:TYR:HE1	1.47	0.80
1:D:4152:ARG:HD2	1:D:4361[B]:TYR:CE2	2.17	0.79
1:A:1361:TYR:H	1:A:1361:TYR:HD2	1.28	0.79
1:D:4150:VAL:HB	1:D:4361[B]:TYR:HE1	1.49	0.77
1:C:3345:THR:HA	6:C:7046:HOH:O	1.83	0.77
1:B:2228[A]:LEU:HG	1:B:2230[A]:PRO:HD3	1.68	0.75
1:D:4034:GLU:HG2	1:D:4042[A]:ARG:HE	1.52	0.75
1:A:1069:ILE:HG23	1:A:1328:MET:SD	2.27	0.74
1:D:4302:GLY:HA3	4:D:8001[B]:13P:H12	1.68	0.74
1:B:2230[B]:PRO:HB2	6:B:6071:HOH:O	1.88	0.74
1:B:2230[A]:PRO:HB2	6:B:6071:HOH:O	1.88	0.74
3:B:6001:2FP:H4	6:B:6797:HOH:O	1.88	0.74
1:B:2294:PRO:HA	6:B:6677:HOH:O	1.87	0.74
1:B:2270:LEU:HB2	3:B:6001:2FP:H3	1.70	0.74
1:C:3302[B]:GLY:HA3	4:C:7001:13P:H12	1.70	0.73
1:C:3237:HIS:O	1:C:3356:LEU:HD21	1.89	0.73
4:D:8002[A]:13P:C1	6:D:8919:HOH:O	2.36	0.72
4:D:8002[A]:13P:H11	6:D:8919:HOH:O	1.89	0.72
1:B:2228[B]:LEU:HG	1:B:2230[B]:PRO:HD3	1.72	0.72
4:D:8002[A]:13P:H31	6:D:8887:HOH:O	1.88	0.71
1:B:2271:SER:O	1:B:2274:MET:HG2	1.90	0.71
1:D:4069:ILE:HD13	1:D:4102:ILE:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3354:GLN:HB2	6:C:7069:HOH:O	1.91	0.70
1:D:4150:VAL:HB	1:D:4361[B]:TYR:CE1	2.27	0.70
1:D:4150:VAL:HB	1:D:4361[A]:TYR:CE1	2.26	0.70
1:D:4191:ILE:HD13	1:D:4361[B]:TYR:HA	1.74	0.69
1:D:4042[A]:ARG:CG	1:D:4042[A]:ARG:HH11	1.91	0.69
1:B:2242:LYS:HE3	1:B:2350:ALA:HB3	1.74	0.69
1:C:3302[A]:GLY:HA3	4:C:7001:13P:H12	1.74	0.68
4:D:8002[A]:13P:C2	6:D:8919:HOH:O	2.40	0.68
1:B:2229[B]:LYS:HD2	1:B:2300[B]:SER:HB3	1.76	0.68
1:D:4038:THR:CG2	1:D:4042[A]:ARG:NH2	2.57	0.68
1:D:4361[A]:TYR:HD2	6:D:8506:HOH:O	1.78	0.67
1:B:2053:GLU:HG3	1:C:3053:GLU:CG	2.24	0.67
1:B:2354:GLN:NE2	6:B:6447:HOH:O	2.30	0.65
1:B:2170:LEU:HG	1:B:2186[A]:VAL:HG13	1.77	0.65
1:A:1353:THR:HB	6:A:5700:HOH:O	1.96	0.65
3:B:6001:2FP:C6	6:B:6799:HOH:O	2.44	0.65
1:D:4301:TYR:HB3	1:D:4304:ALA:HB3	1.78	0.65
1:A:1339:LYS:HE2	1:A:1339:LYS:HA	1.79	0.65
1:C:3271:SER:O	1:C:3274:MET:HB2	1.97	0.65
1:D:4042[B]:ARG:O	1:D:4045:ARG:HB3	1.97	0.65
1:B:2146[A]:LYS:NZ	6:B:6795:HOH:O	2.30	0.65
1:B:2362:THR:HG22	1:B:2363:TYR:H	1.63	0.64
1:C:3346:GLY:HA2	6:C:7648:HOH:O	1.96	0.64
1:B:2044:GLN:HG2	6:B:6326:HOH:O	1.96	0.64
1:A:1317:ALA:HB2	6:A:5588:HOH:O	1.97	0.64
1:B:2170:LEU:HG	1:B:2186[B]:VAL:HG13	1.78	0.64
1:B:2229[A]:LYS:HE2	6:B:6801:HOH:O	1.97	0.64
1:D:4076:VAL:HG22	6:D:8492:HOH:O	1.98	0.63
1:C:3045[A]:ARG:HB3	6:C:7092:HOH:O	1.99	0.63
1:A:1254:THR:O	1:A:1258:ARG:HG3	1.99	0.63
1:C:3321:LYS:HE3	6:C:7369:HOH:O	1.97	0.63
1:C:3045[B]:ARG:HB3	6:C:7092:HOH:O	1.99	0.62
1:A:1361:TYR:N	1:A:1361:TYR:CD2	2.67	0.62
1:A:1280:THR:HG21	1:A:1333:VAL:CG1	2.29	0.62
1:A:1069:ILE:HD13	1:A:1102:ILE:HD11	1.80	0.62
1:A:1357:PHE:O	1:A:1358:THR:HB	1.99	0.62
1:A:1361:TYR:N	1:A:1361:TYR:HD2	1.96	0.62
1:D:4352:SER:HA	6:D:8468:HOH:O	1.98	0.61
1:D:4148:ARG:NH1	1:D:4363[A]:TYR:O	2.34	0.61
1:B:2164:GLN:HG2	6:B:6175:HOH:O	2.01	0.61
1:B:2353:THR:HG22	1:B:2355:SER:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:SER:O	1:A:1274:MET:HB2	2.01	0.60
1:B:2358:THR:HG23	6:B:6779:HOH:O	2.02	0.59
1:D:4362[B]:THR:HG22	6:D:8407:HOH:O	2.02	0.59
1:A:1353:THR:HG22	1:A:1353:THR:O	2.02	0.59
1:B:2069:ILE:HD11	1:B:2100:LYS:HD3	1.85	0.59
1:D:4254:THR:O	1:D:4258:ARG:HG3	2.03	0.59
1:C:3036:VAL:HG13	1:C:3055:ARG:NH1	2.17	0.58
1:A:1146:LYS:HE2	1:A:1187:GLU:OE2	2.03	0.58
1:C:3192:PRO:HB2	1:C:3237:HIS:CD2	2.38	0.58
1:C:3089:GLN:HG3	6:C:7602:HOH:O	2.03	0.58
1:A:1046:ILE:HD13	1:A:1310:LEU:HG	1.86	0.58
1:B:2053:GLU:HG2	6:B:6509:HOH:O	2.04	0.57
1:B:2242:LYS:HE3	1:B:2350:ALA:CB	2.33	0.57
1:B:2320:LYS:O	1:B:2324:GLN:HG3	2.05	0.56
1:A:1021:ARG:HD3	6:A:5750:HOH:O	2.06	0.56
1:D:4191:ILE:HD13	1:D:4361[A]:TYR:HA	1.87	0.56
1:D:4191:ILE:CD1	1:D:4361[B]:TYR:HA	2.35	0.56
1:B:2146[A]:LYS:CG	6:B:6801:HOH:O	2.40	0.56
3:B:6001:2FP:H62	6:B:6799:HOH:O	2.05	0.55
1:D:4361[B]:TYR:HD2	6:D:8506:HOH:O	1.88	0.55
1:B:2166:ASN:O	1:B:2170:LEU:HB2	2.06	0.55
1:D:4076:VAL:HG23	1:D:4102:ILE:HG21	1.89	0.55
1:B:2252:THR:HG23	6:B:6546:HOH:O	2.06	0.55
1:B:2053:GLU:CG	1:C:3053:GLU:HG3	2.29	0.55
1:C:3061:ILE:HG23	1:C:3320:LYS:HG3	1.89	0.55
1:C:3152:ARG:HB3	1:C:3191:ILE:HD11	1.89	0.55
1:C:3330:ARG:NH1	1:C:3333:VAL:HG21	2.21	0.55
1:D:4219:HIS:HD2	6:D:8698:HOH:O	1.90	0.55
1:C:3276:GLU:HG3	6:C:7625:HOH:O	2.05	0.55
1:C:3069:ILE:HD13	1:C:3328:MET:SD	2.46	0.54
1:C:3362:THR:HG22	1:C:3363:TYR:HD1	1.73	0.54
1:D:4042[B]:ARG:HB3	1:D:4310:LEU:HD21	1.89	0.54
1:D:4034:GLU:HB2	1:D:4039:MET:HG2	1.90	0.54
1:B:2354:GLN:O	1:B:2354:GLN:HG2	2.08	0.54
1:B:2229[A]:LYS:CE	6:B:6801:HOH:O	2.54	0.53
1:A:1204:VAL:O	1:A:1208:VAL:HG13	2.07	0.53
1:B:2148:ARG:HD2	3:B:6001:2FP:H5	1.90	0.53
1:D:4106:ILE:HG22	1:D:4142:VAL:HG11	1.91	0.53
1:A:1333:VAL:HG13	1:A:1342:TYR:CE1	2.44	0.53
1:B:2046:ILE:HD13	1:B:2310:LEU:HD22	1.91	0.53
1:B:2344:HIS:HB3	6:B:6402:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3242:LYS:HE2	6:C:7513:HOH:O	2.09	0.53
1:B:2033[B]:ASP:OD2	1:B:2146[B]:LYS:HD2	2.09	0.52
1:B:2033[A]:ASP:OD2	1:B:2146[A]:LYS:HE2	2.08	0.52
1:C:3250:MET:O	1:C:3254:THR:HG23	2.09	0.52
1:C:3042[B]:ARG:HD2	1:C:3303[B]:ARG:CZ	2.39	0.52
1:B:2356:LEU:HG	1:B:2356:LEU:O	2.09	0.52
1:C:3046[B]:ILE:HG22	6:C:7873:HOH:O	2.08	0.52
1:C:3345:THR:HG21	6:C:7207:HOH:O	2.08	0.52
1:D:4228:LEU:HG	1:D:4230:PRO:HD3	1.90	0.52
1:C:3146[B]:LYS:NZ	6:C:7898:HOH:O	0.67	0.52
1:C:3046[A]:ILE:HG22	6:C:7873:HOH:O	2.09	0.52
1:D:4042[B]:ARG:NH2	6:D:8922:HOH:O	2.41	0.52
1:A:1088:SER:HB2	6:A:5598:HOH:O	2.09	0.52
1:D:4355:SER:HA	6:D:8201:HOH:O	2.10	0.52
1:D:4152:ARG:HD2	1:D:4361[A]:TYR:CE2	2.44	0.52
1:D:4150:VAL:CB	1:D:4361[B]:TYR:HE1	2.21	0.52
1:B:2065:VAL:HG23	1:B:2069:ILE:HG12	1.92	0.51
1:A:1280:THR:HG21	1:A:1333:VAL:HG12	1.91	0.51
1:C:3358:THR:O	1:C:3358:THR:HG22	2.10	0.51
1:D:4071:GLN:HG2	6:D:8668:HOH:O	2.09	0.51
1:A:1069:ILE:HD11	1:A:1100:LYS:HD3	1.93	0.51
1:C:3330:ARG:HH21	1:C:3330:ARG:HG3	1.76	0.51
1:A:1018:ILE:O	1:A:1022:ILE:HG13	2.10	0.51
1:C:3301:TYR:HB3	1:C:3304[B]:ALA:HB3	1.93	0.51
1:C:3213:TYR:OH	1:C:3228[A]:LEU:HG	2.11	0.50
1:A:1106:ILE:HG22	1:A:1142:VAL:HG11	1.93	0.50
1:A:1351:ALA:HB1	1:A:1354:GLN:HB2	1.94	0.50
4:D:8002[A]:13P:H12	6:D:8928:HOH:O	2.11	0.50
1:A:1198:LEU:HD12	1:A:1233:VAL:HG12	1.92	0.50
1:A:1271:SER:HB2	6:A:5458:HOH:O	2.11	0.50
1:B:2358:THR:O	1:B:2359:ALA:HB2	2.11	0.50
1:B:2362:THR:HG22	1:B:2363:TYR:N	2.27	0.50
1:D:4034:GLU:HG2	1:D:4042[A]:ARG:NE	2.24	0.50
1:D:4038:THR:HG22	1:D:4042[A]:ARG:NH2	2.27	0.50
1:A:1208:VAL:O	1:A:1212:VAL:HG23	2.12	0.50
1:B:2148:ARG:HD3	5:B:6003:G3P:C1	2.39	0.50
1:D:4069:ILE:HD11	1:D:4100:LYS:HD3	1.94	0.50
1:A:1228:LEU:HG	1:A:1230:PRO:HD3	1.93	0.49
1:A:1067:ASN:HD22	1:A:1100:LYS:HG2	1.76	0.49
1:A:1233:VAL:O	1:A:1248:VAL:HG13	2.12	0.49
1:A:1351:ALA:O	1:A:1352:SER:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4363[B]:TYR:HD2	6:D:8916:HOH:O	1.44	0.49
1:A:1329:LYS:HE3	6:A:5666:HOH:O	2.12	0.49
1:B:2277:GLU:OE2	1:B:2354:GLN:NE2	2.46	0.49
1:D:4186:VAL:HG12	1:D:4188:PRO:HD3	1.93	0.49
1:C:3186:VAL:HG12	1:C:3188:PRO:HD3	1.94	0.49
1:A:1311:ALA:HB1	6:A:5657:HOH:O	2.13	0.49
1:B:2223:LEU:HD11	6:B:6359:HOH:O	2.11	0.49
1:B:2229[B]:LYS:HD2	1:B:2300[B]:SER:CB	2.41	0.49
1:C:3083:LEU:HD22	1:C:3094:ARG:HD3	1.93	0.49
1:B:2303[A]:ARG:HG2	6:B:6768:HOH:O	2.13	0.49
1:C:3329:LYS:O	1:C:3332:VAL:HG22	2.13	0.49
1:B:2083:LEU:O	1:B:2083:LEU:HD22	2.13	0.48
1:B:2358:THR:HA	6:B:6779:HOH:O	2.13	0.48
1:C:3276:GLU:CD	1:C:3330:ARG:HD3	2.34	0.48
1:B:2069:ILE:HD13	1:B:2102:ILE:HD11	1.95	0.48
1:D:4066:ASP:O	1:D:4069:ILE:HG13	2.13	0.48
1:A:1075:GLY:HA2	1:A:1103:VAL:O	2.13	0.48
1:C:3228[B]:LEU:HD13	1:C:3230[B]:PRO:HD3	1.94	0.48
1:D:4120:LYS:O	1:D:4361[A]:TYR:HE2	1.97	0.48
1:D:4362[A]:THR:O	1:D:4363[A]:TYR:HD1	1.96	0.48
1:A:1356:LEU:HD13	6:A:5494:HOH:O	2.14	0.48
1:D:4081:GLU:HG3	1:D:4082:THR:N	2.28	0.48
1:C:3173:TYR:CE1	1:C:3177:CYS:SG	3.06	0.48
1:C:3349:GLY:HA2	6:C:7764:HOH:O	2.14	0.47
1:D:4047:LYS:HG2	6:D:8114:HOH:O	2.13	0.47
1:B:2358:THR:O	1:B:2359:ALA:CB	2.63	0.47
1:C:3276:GLU:HB3	1:C:3330:ARG:NH2	2.29	0.47
1:B:2358:THR:HG23	6:B:6780:HOH:O	2.13	0.47
1:A:1286:ILE:HG22	1:A:1297:LEU:HD13	1.97	0.47
1:B:2270:LEU:HB2	4:B:6002:13P:O3P	2.15	0.47
1:C:3349:GLY:HA3	6:C:7263:HOH:O	2.14	0.47
1:D:4204:VAL:O	1:D:4208:VAL:HG23	2.14	0.47
1:A:1067:ASN:ND2	1:A:1100:LYS:HE2	2.29	0.47
1:B:2229[B]:LYS:HD3	6:B:6801:HOH:O	2.14	0.47
1:B:2354:GLN:C	1:B:2356:LEU:N	2.68	0.47
1:B:2146[B]:LYS:HE2	1:B:2187[B]:GLU:OE2	2.15	0.47
1:B:2089:GLN:HG2	6:B:6100:HOH:O	2.14	0.46
1:C:3301:TYR:HB3	1:C:3304[A]:ALA:HB3	1.97	0.46
1:C:3330:ARG:HG3	1:C:3330:ARG:NH2	2.30	0.46
1:D:4079:PHE:HD1	1:D:4081:GLU:HG2	1.79	0.46
1:C:3357:PHE:HB3	1:C:3359:ALA:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4360[A]:SER:OG	1:D:4361[A]:TYR:N	2.49	0.46
1:A:1063:PHE:CD1	1:A:1063:PHE:N	2.82	0.46
1:A:1065:VAL:HG23	1:A:1324:GLN:HB3	1.97	0.46
1:B:2039:MET:SD	1:B:2059:ARG:NH2	2.88	0.46
1:B:2237:HIS:HE1	6:B:6531:HOH:O	1.99	0.46
1:D:4148:ARG:HH12	1:D:4362[B]:THR:C	2.19	0.46
1:B:2047:LYS:HB3	6:B:6543:HOH:O	2.15	0.45
1:C:3213:TYR:OH	1:C:3228[B]:LEU:HG	2.15	0.45
1:D:4191:ILE:CD1	1:D:4361[A]:TYR:HA	2.45	0.45
1:C:3302[A]:GLY:CA	4:C:7001:13P:H12	2.44	0.45
1:B:2146[B]:LYS:HG3	6:B:6801:HOH:O	2.16	0.45
1:B:2212:VAL:HG13	6:B:6701:HOH:O	2.15	0.45
1:C:3350:ALA:HB2	6:C:7379:HOH:O	2.16	0.45
1:B:2066:ASP:HB2	1:B:2328:MET:HE1	1.98	0.45
1:D:4350:ALA:O	1:D:4351:ALA:HB3	2.17	0.45
1:B:2354:GLN:CG	1:B:2354:GLN:O	2.64	0.45
1:D:4148:ARG:NH2	1:D:4363[B]:TYR:HA	2.31	0.45
1:D:4202:GLN:HB2	1:D:4233:VAL:HG11	1.99	0.45
4:D:8001[B]:13P:H31	6:D:8925:HOH:O	2.16	0.45
1:C:3167:ALA:HB1	1:C:3212:VAL:HA	1.99	0.45
1:D:4120:LYS:HB3	6:D:8506:HOH:O	2.17	0.45
1:D:4271:SER:HB2	6:D:8693:HOH:O	2.17	0.45
1:A:1295:TRP:CZ3	1:A:1297:LEU:HD21	2.52	0.44
1:A:1361:TYR:HB2	1:A:1362:THR:H	1.61	0.44
1:D:4076:VAL:HG23	1:D:4102:ILE:CG2	2.47	0.44
1:A:1202:GLN:HB2	1:A:1233:VAL:HG11	1.98	0.44
1:B:2040:GLY:O	1:B:2044:GLN:HB2	2.17	0.44
1:D:4360[B]:SER:O	1:D:4361[B]:TYR:CB	2.65	0.44
3:A:5001:2FP:O4	3:A:5001:2FP:H11	2.18	0.44
1:B:2207:LYS:HE2	6:B:6259:HOH:O	2.16	0.44
1:B:2150:VAL:HG13	1:B:2191:ILE:HG23	2.00	0.44
1:C:3303[B]:ARG:HB2	4:C:7001:13P:O3P	2.17	0.44
1:D:4150:VAL:CB	1:D:4361[A]:TYR:HE1	2.25	0.44
1:B:2144:PHE:HB2	1:B:2183:VAL:O	2.18	0.44
1:C:3151:LEU:HD11	6:C:7253:HOH:O	2.16	0.44
1:A:1028:GLY:HA3	1:A:1299:PHE:CZ	2.52	0.44
1:A:1078:LEU:O	1:A:1106:ILE:HD12	2.18	0.43
1:B:2249:ALA:O	1:B:2253:VAL:HG23	2.19	0.43
1:B:2354:GLN:C	1:B:2356:LEU:H	2.21	0.43
1:B:2066:ASP:O	1:B:2069:ILE:HG13	2.18	0.43
6:C:7907:HOH:O	1:D:4206:GLU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:ARG:HD2	6:A:5294:HOH:O	2.18	0.43
1:B:2106:ILE:HG22	1:B:2142:VAL:HG11	2.00	0.43
1:C:3359:ALA:O	1:C:3360:SER:OG	2.32	0.43
1:D:4045:ARG:O	1:D:4045:ARG:HG2	2.18	0.43
1:D:4360[B]:SER:OG	1:D:4361[B]:TYR:N	2.51	0.43
1:C:3224:GLU:OE2	1:D:4258:ARG:HD3	2.18	0.43
1:D:4021:ARG:HD3	6:D:8574:HOH:O	2.18	0.43
1:D:4363[B]:TYR:HE1	6:D:8917:HOH:O	1.76	0.43
1:C:3249:ALA:HB1	1:C:3286:ILE:HA	2.01	0.43
1:B:2272:GLY:HA2	6:B:6782:HOH:O	2.17	0.43
1:C:3241:LYS:HD3	6:C:7372:HOH:O	2.19	0.42
1:A:1066:ASP:O	1:A:1069:ILE:HG13	2.19	0.42
1:A:1164:GLN:HB2	1:A:1164:GLN:HE21	1.55	0.42
1:A:1214:LYS:HG2	1:B:2214:LYS:HG2	2.00	0.42
1:B:2065:VAL:CG2	1:B:2069:ILE:HG12	2.49	0.42
1:B:2348:SER:OG	1:B:2349:GLY:N	2.53	0.42
1:D:4038:THR:CG2	1:D:4042[A]:ARG:HH21	2.31	0.42
1:D:4280:THR:HG21	1:D:4333:VAL:HG13	2.01	0.42
1:A:1144:PHE:HB2	1:A:1183:VAL:O	2.18	0.42
1:A:1148:ARG:HD3	3:A:5001:2FP:O62	2.19	0.42
1:C:3358:THR:O	1:C:3358:THR:CG2	2.68	0.42
1:D:4241:LYS:HE2	6:D:8342:HOH:O	2.18	0.42
1:B:2015:LEU:HB3	1:B:2225:GLY:HA3	2.02	0.42
1:D:4042[A]:ARG:NH1	1:D:4042[A]:ARG:CG	2.59	0.42
1:B:2049:GLU:HG3	1:C:3088:SER:O	2.20	0.42
1:D:4229:LYS:HA	1:D:4268:CYS:O	2.20	0.42
1:D:4038:THR:O	1:D:4041[A]:ASN:HB2	2.20	0.42
1:C:3078:LEU:O	1:C:3106:ILE:HD12	2.20	0.42
1:D:4357:PHE:HE1	6:D:8096:HOH:O	2.02	0.42
1:C:3081:GLU:HG3	6:C:7805:HOH:O	2.19	0.42
1:B:2047:LYS:HD3	1:B:2047:LYS:N	2.35	0.41
1:B:2222:TYR:CZ	1:B:2224:GLU:HB2	2.54	0.41
1:D:4018:ILE:O	1:D:4022:ILE:HG13	2.20	0.41
1:B:2069:ILE:HD11	1:B:2100:LYS:CD	2.49	0.41
1:B:2146[A]:LYS:HB3	1:B:2146[A]:LYS:HE3	1.71	0.41
1:D:4168:ASN:OD1	1:D:4219:HIS:HE1	2.02	0.41
1:D:4295:TRP:O	1:D:4297:LEU:HD22	2.19	0.41
1:A:1155:ASP:O	1:A:1156:GLN:HB2	2.21	0.41
1:A:1229:LYS:HA	1:A:1268:CYS:O	2.21	0.41
1:C:3061:ILE:HG21	1:C:3323:THR:HB	2.03	0.41
1:C:3144:PHE:HB2	1:C:3183:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4152:ARG:HD2	1:D:4361[B]:TYR:HE2	1.79	0.41
1:D:4150:VAL:CB	1:D:4361[B]:TYR:CE1	3.01	0.41
1:A:1360:SER:O	1:A:1361:TYR:C	2.59	0.41
1:B:2352:SER:HB2	6:B:6580:HOH:O	2.20	0.41
1:A:1021:ARG:HG2	6:A:5765:HOH:O	2.19	0.41
1:A:1087:ASP:OD2	1:A:1091:LYS:HB2	2.21	0.41
1:A:1113:ALA:HA	1:A:1114:PRO:HD3	1.90	0.41
1:A:1205:THR:O	1:A:1208:VAL:HG22	2.20	0.41
1:A:1207:LYS:HE2	6:A:5213:HOH:O	2.21	0.41
1:B:2354:GLN:O	1:B:2356:LEU:N	2.54	0.41
1:B:2356:LEU:O	1:B:2356:LEU:CG	2.69	0.41
1:D:4360[B]:SER:O	1:D:4361[B]:TYR:HB2	2.21	0.41
1:A:1223:LEU:HD13	6:A:5079:HOH:O	2.20	0.41
1:D:4030:LEU:HB3	6:D:8492:HOH:O	2.20	0.41
1:D:4355:SER:HB3	6:D:8790:HOH:O	2.20	0.41
1:C:3130:LEU:HD22	1:C:3134:CYS:SG	2.62	0.40
1:B:2207:LYS:HD3	1:B:2207:LYS:HA	1.87	0.40
1:D:4069:ILE:HD12	1:D:4070:ASN:N	2.35	0.40
1:A:1119:ASN:O	1:A:1152:ARG:NH1	2.54	0.40
1:B:2279:ALA:O	1:B:2283:LEU:HB2	2.20	0.40
1:C:3208:VAL:O	1:C:3212:VAL:HG23	2.21	0.40
1:C:3222:TYR:CZ	1:C:3224:GLU:HB2	2.56	0.40
1:C:3357:PHE:HE1	6:C:7069:HOH:O	2.03	0.40
1:D:4124:ILE:HG13	1:D:4149:ALA:HA	2.02	0.40
1:D:4264:VAL:HA	1:D:4265:PRO:HD3	1.89	0.40
1:B:2015:LEU:HD12	1:B:2015:LEU:HA	1.96	0.40
1:C:3358:THR:HG23	6:C:7065:HOH:O	2.21	0.40
1:D:4173:TYR:CE1	1:D:4177:CYS:SG	3.14	0.40
1:C:3263:ALA:HB2	1:D:4258:ARG:HG2	2.02	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	367/363 (101%)	337 (92%)	22 (6%)	8 (2%)	6	2
1	B	379/363 (104%)	352 (93%)	20 (5%)	7 (2%)	8	4
1	C	378/363 (104%)	356 (94%)	17 (4%)	5 (1%)	12	7
1	D	369/363 (102%)	343 (93%)	22 (6%)	4 (1%)	14	9
All	All	1493/1452 (103%)	1388 (93%)	81 (5%)	24 (2%)	9	5

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1344	HIS
1	A	1353	THR
1	A	1361	TYR
1	B	2357	PHE
1	B	2359	ALA
1	B	2360	SER
1	C	3350	ALA
1	D	4361[A]	TYR
1	D	4361[B]	TYR
1	A	1352	SER
1	A	1358	THR
1	B	2351	ALA
1	B	2353	THR
1	B	2355	SER
1	C	3349	GLY
1	A	1351	ALA
1	A	1355	SER
1	B	2362	THR
1	C	3355	SER
1	C	3360	SER
1	D	4350	ALA
1	D	4355	SER
1	C	3356	LEU
1	A	1362	THR

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	297/293 (101%)	280 (94%)	17 (6%)	20	18
1	B	307/293 (105%)	293 (95%)	14 (5%)	27	26
1	C	307/293 (105%)	287 (94%)	20 (6%)	17	14
1	D	301/293 (103%)	273 (91%)	28 (9%)	9	6
All	All	1212/1172 (103%)	1133 (94%)	79 (6%)	17	14

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1070	ASN
1	A	1083	LEU
1	A	1131	SER
1	A	1152	ARG
1	A	1161	LEU
1	A	1164	GLN
1	A	1173	TYR
1	A	1223	LEU
1	A	1230	PRO
1	A	1256	LEU
1	A	1257	HIS
1	A	1295	TRP
1	A	1316	LYS
1	A	1318	GLU
1	A	1357	PHE
1	A	1361	TYR
1	A	1363	TYR
1	B	2015	LEU
1	B	2041	ASN
1	B	2070	ASN
1	B	2083	LEU
1	B	2127	LEU
1	B	2173	TYR
1	B	2283	LEU
1	B	2295	TRP
1	B	2310	LEU
1	B	2321	LYS
1	B	2352	SER
1	B	2353	THR
1	B	2355	SER
1	B	2357	PHE
1	C	3053	GLU
1	C	3070	ASN

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Mol	Chain	Res	Type
1	C	3130	LEU
1	C	3173	TYR
1	C	3228[A]	LEU
1	C	3228[B]	LEU
1	C	3230[A]	PRO
1	C	3230[B]	PRO
1	C	3240	THR
1	C	3246	GLU
1	C	3256	LEU
1	C	3257	HIS
1	C	3271	SER
1	C	3283	LEU
1	C	3295	TRP
1	C	3330	ARG
1	C	3352	SER
1	C	3354	GLN
1	C	3355	SER
1	C	3356	LEU
1	D	4007	LEU
1	D	4042[A]	ARG
1	D	4042[B]	ARG
1	D	4044	GLN
1	D	4045	ARG
1	D	4067	ASN
1	D	4070	ASN
1	D	4099	GLU
1	D	4108	LEU
1	D	4127	LEU
1	D	4130	LEU
1	D	4131	SER
1	D	4136	GLN
1	D	4150	VAL
1	D	4152	ARG
1	D	4156	GLN
1	D	4161	LEU
1	D	4172	ARG
1	D	4173	TYR
1	D	4214	LYS
1	D	4242	LYS
1	D	4271	SER
1	D	4281	LEU
1	D	4295	TRP

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Mol	Chain	Res	Type
1	D	4333	VAL
1	D	4353	THR
1	D	4361[A]	TYR
1	D	4361[B]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1020	GLN
1	A	1067	ASN
1	A	1070	ASN
1	A	1089	GLN
1	A	1156	GLN
1	A	1168	ASN
1	A	1202	GLN
1	A	1257	HIS
1	A	1336	GLN
1	B	2070	ASN
1	B	2110	GLN
1	B	2164	GLN
1	B	2220	HIS
1	B	2237	HIS
1	B	2354	GLN
1	C	3070	ASN
1	C	3089	GLN
1	D	4070	ASN
1	D	4095	ASN
1	D	4156	GLN
1	D	4168	ASN
1	D	4219	HIS
1	D	4334	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	13P	C	7001	-	9,9,9	1.14	1 (11%)	10,12,12	1.51	2 (20%)
2	SO4	B	6000	-	4,4,4	0.59	0	6,6,6	0.28	0
2	SO4	A	5000	-	4,4,4	0.45	0	6,6,6	0.15	0
4	13P	D	8002[A]	-	9,9,9	1.06	1 (11%)	10,12,12	1.46	2 (20%)
3	2FP	B	6001	1,5,4	18,19,19	1.05	1 (5%)	21,28,28	2.05	9 (42%)
5	G3P	B	6003	3	9,9,9	2.08	2 (22%)	11,12,12	1.14	1 (9%)
3	2FP	A	5001	-	18,19,19	1.18	2 (11%)	21,28,28	1.56	6 (28%)
4	13P	D	8001[B]	-	9,9,9	1.13	1 (11%)	10,12,12	1.41	2 (20%)
4	13P	B	6002	3	9,9,9	1.09	1 (11%)	10,12,12	1.21	1 (10%)
2	SO4	C	7000	-	4,4,4	0.54	0	6,6,6	0.25	0
2	SO4	D	8000	-	4,4,4	0.65	0	6,6,6	0.25	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
4	13P	C	7001	-	-	2/7/8/8	-
4	13P	D	8002[A]	-	-	7/7/8/8	-
3	2FP	B	6001	1,5,4	2/2/6/6	16/24/24/24	-
5	G3P	B	6003	3	1/1/2/2	4/8/8/8	-
3	2FP	A	5001	-	2/2/6/6	15/24/24/24	-
4	13P	D	8001[B]	-	-	6/7/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	13P	B	6002	3	-	2/7/8/8	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	6003	G3P	O1-C1	-4.95	1.21	1.42
5	B	6003	G3P	P-O2P	2.94	1.60	1.50
4	D	8001[B]	13P	P-O1P	2.80	1.59	1.50
4	B	6002	13P	P-O1P	2.50	1.58	1.50
3	A	5001	2FP	O2-C2	2.47	1.25	1.21
4	C	7001	13P	P-O1P	2.47	1.58	1.50
4	D	8002[A]	13P	P-O1P	2.39	1.58	1.50
3	A	5001	2FP	C4-C3	2.34	1.59	1.53
3	B	6001	2FP	P6-O63	2.25	1.57	1.50

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6001	2FP	O13-P1-O1	3.87	117.04	106.73
3	B	6001	2FP	O12-P1-O11	-3.85	95.59	110.68
3	B	6001	2FP	O6-P6-O63	3.39	115.98	106.47
5	B	6003	G3P	O1-C1-C2	3.22	125.63	110.20
3	A	5001	2FP	O4-C4-C3	3.08	114.82	109.21
4	C	7001	13P	O1-P-O1P	3.01	114.93	106.47
4	D	8001[B]	13P	O3P-P-O1	2.99	114.69	106.73
4	D	8002[A]	13P	O2P-P-O1	2.78	114.13	106.73
3	B	6001	2FP	P6-O6-C6	2.52	125.23	118.30
3	B	6001	2FP	O13-P1-O11	-2.41	101.26	110.68
3	A	5001	2FP	O62-P6-O6	2.37	113.05	106.73
3	A	5001	2FP	O12-P1-O1	2.34	112.96	106.73
3	B	6001	2FP	O13-P1-O12	2.31	116.46	107.64
4	B	6002	13P	O2P-P-O1P	-2.23	101.94	110.68
4	D	8001[B]	13P	O2P-P-O1P	-2.22	101.99	110.68
3	A	5001	2FP	O6-P6-O63	2.18	112.60	106.47
3	B	6001	2FP	O4-C4-C5	-2.15	103.61	108.81
3	B	6001	2FP	O12-P1-O1	2.13	112.41	106.73
4	D	8002[A]	13P	O1-P-O1P	2.11	112.41	106.47
3	B	6001	2FP	C6-C5-C4	-2.08	108.19	112.20
3	A	5001	2FP	O4-C4-C5	-2.07	103.81	108.81
3	A	5001	2FP	O12-P1-O11	-2.07	102.58	110.68
4	C	7001	13P	O2P-P-O1	2.05	112.20	106.73

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	6003	G3P	C2
3	B	6001	2FP	C3
3	B	6001	2FP	C4
3	A	5001	2FP	C3
3	A	5001	2FP	C4

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	7001	13P	O2-C2-C3-O3
4	D	8002[A]	13P	C1-O1-P-O2P
4	D	8002[A]	13P	C1-O1-P-O3P
4	D	8002[A]	13P	C2-C1-O1-P
4	D	8002[A]	13P	O2-C2-C3-O3
3	B	6001	2FP	O5-C5-C6-O6
3	B	6001	2FP	C4-C5-C6-O6
3	B	6001	2FP	O3-C3-C4-C5
3	B	6001	2FP	C2-C3-C4-C5
3	B	6001	2FP	O3-C3-C4-O4
3	B	6001	2FP	C2-C3-C4-O4
3	B	6001	2FP	O2-C2-C3-O3
3	B	6001	2FP	O1-C1-C2-C3
3	A	5001	2FP	O5-C5-C6-O6
3	A	5001	2FP	C4-C5-C6-O6
3	A	5001	2FP	O4-C4-C5-C6
3	A	5001	2FP	O4-C4-C5-O5
3	A	5001	2FP	C3-C4-C5-O5
3	A	5001	2FP	C1-C2-C3-C4
3	A	5001	2FP	C2-C1-O1-P1
3	A	5001	2FP	C1-O1-P1-O12
3	A	5001	2FP	C1-O1-P1-O13
4	D	8001[B]	13P	C1-O1-P-O2P
4	D	8001[B]	13P	C1-O1-P-O3P
4	D	8001[B]	13P	O2-C2-C3-O3
3	B	6001	2FP	C5-C6-O6-P6
3	A	5001	2FP	C3-C4-C5-C6
5	B	6003	G3P	O1-C1-C2-O2
5	B	6003	G3P	O2-C2-C3-O1P
4	C	7001	13P	O1-C1-C2-O2
4	D	8002[A]	13P	O1-C1-C2-O2
4	D	8001[B]	13P	O1-C1-C2-O2
4	B	6002	13P	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	6001	2FP	C3-C4-C5-C6
5	B	6003	G3P	C1-C2-C3-O1P
5	B	6003	G3P	O1-C1-C2-C3
3	B	6001	2FP	O4-C4-C5-C6
3	A	5001	2FP	C1-O1-P1-O11
4	D	8001[B]	13P	C1-O1-P-O1P
3	B	6001	2FP	C6-O6-P6-O62
3	A	5001	2FP	O2-C2-C3-C4
3	B	6001	2FP	C3-C4-C5-O5
4	D	8002[A]	13P	C1-O1-P-O1P
3	B	6001	2FP	C6-O6-P6-O63
3	A	5001	2FP	C6-O6-P6-O63
3	B	6001	2FP	O4-C4-C5-O5
4	D	8002[A]	13P	O1-C1-C2-C3
4	B	6002	13P	O1-C1-C2-C3
3	A	5001	2FP	C5-C6-O6-P6
3	A	5001	2FP	C6-O6-P6-O62
3	B	6001	2FP	C2-C1-O1-P1
4	D	8001[B]	13P	O1-C1-C2-C3

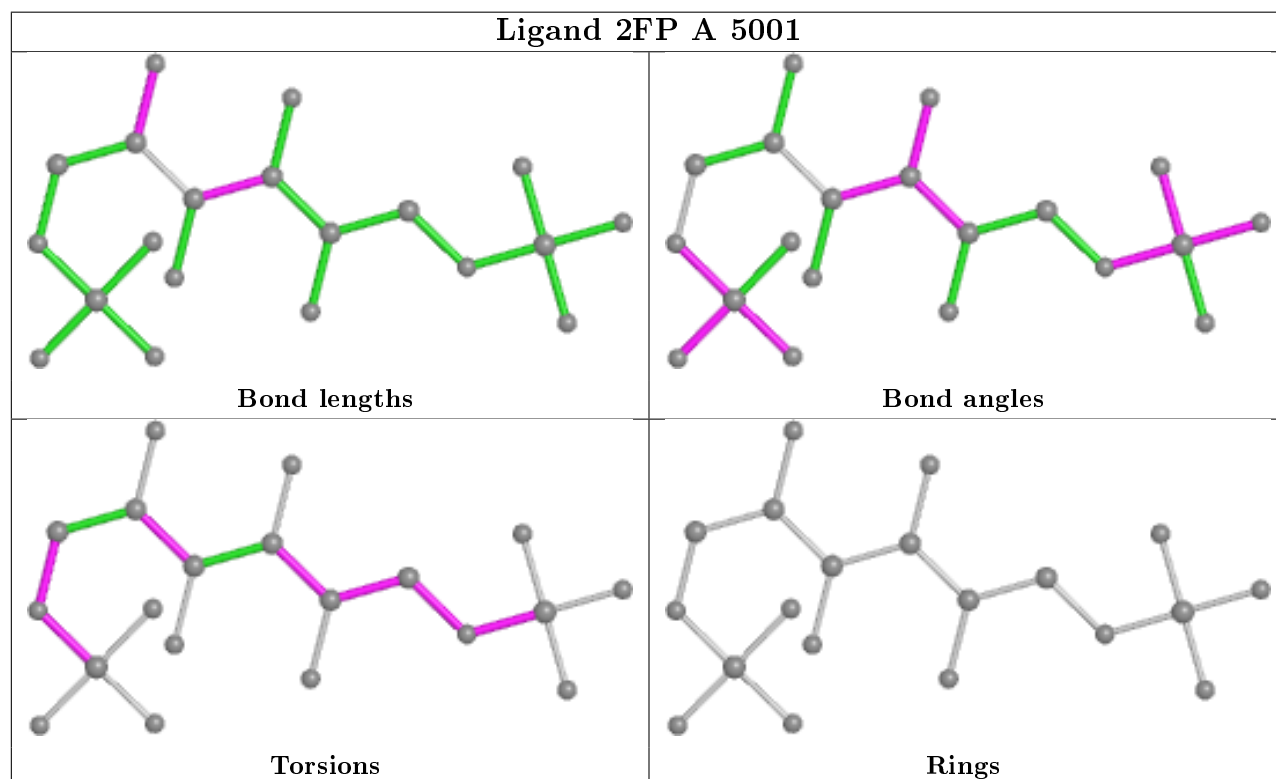
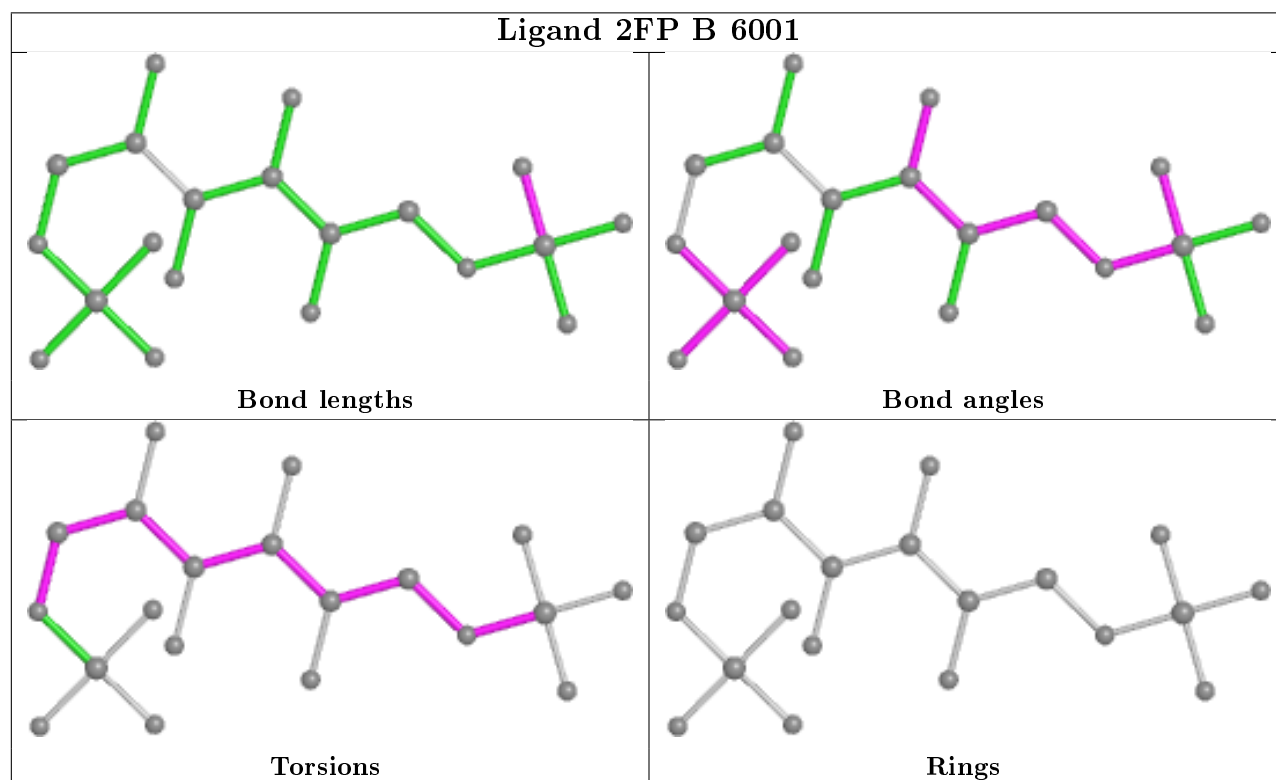
There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	7001	13P	6	0
4	D	8002[A]	13P	5	0
3	B	6001	2FP	5	0
5	B	6003	G3P	3	0
3	A	5001	2FP	2	0
4	D	8001[B]	13P	2	0
4	B	6002	13P	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.