



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2020 – 12:24 PM EDT

PDB ID : 3C6O
Title : Small molecule agonists and antagonists of F-box protein-substrate interactions in auxin perception and signaling
Authors : Tan, X.
Deposited on : 2008-02-04
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

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 : 2.14.6
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) : 2.14.6

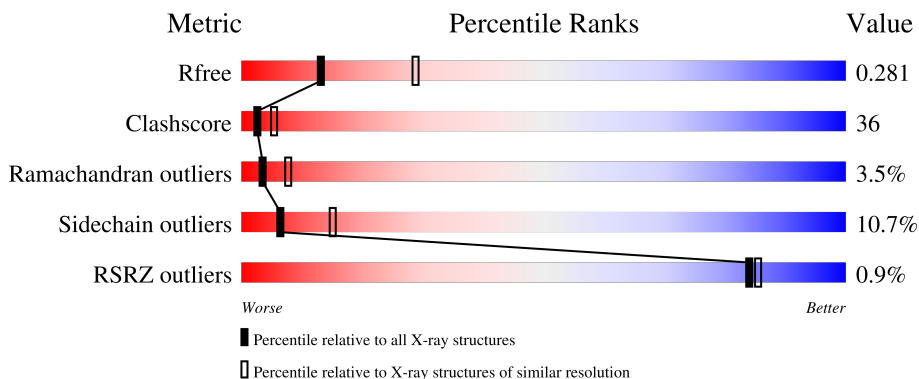
1 Overall quality at a glance

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 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	160	
2	B	594	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5358 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.

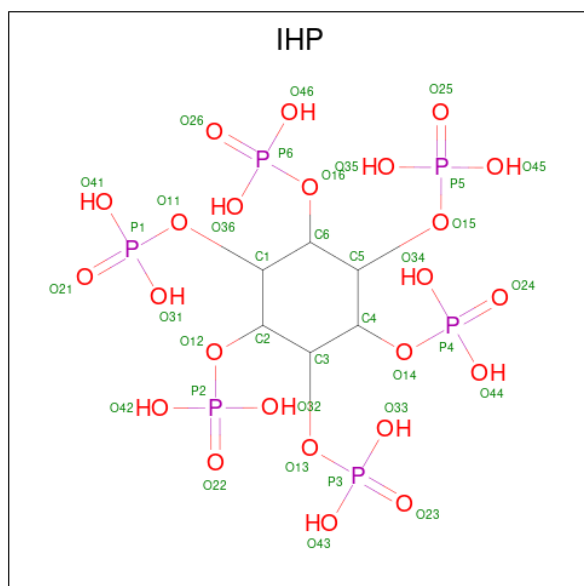
- Molecule 1 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	76	Total	C	N	O	S	0	0	0
			618	393	100	123	2			

- Molecule 2 is a protein called TRANSPORT INHIBITOR RESPONSE 1.

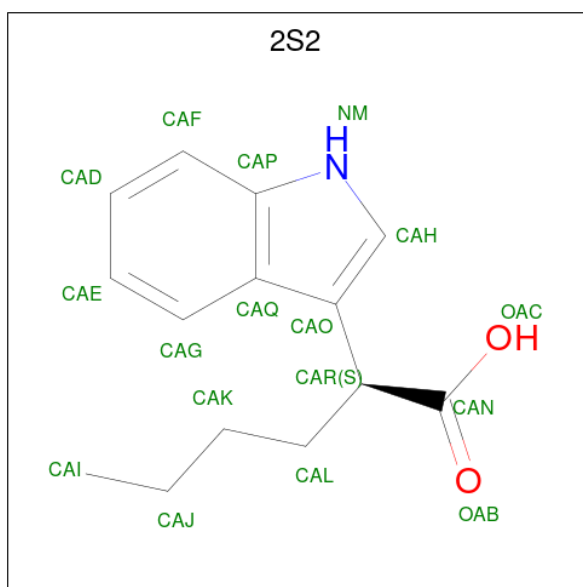
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	567	Total	C	N	O	S	0	0	0
			4461	2850	754	820	37			

- Molecule 3 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			36	6	24	6		

- Molecule 4 is (2S)-2-(1H-indol-3-yl)hexanoic acid (three-letter code: 2S2) (formula: $C_{14}H_{17}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			17	14	1	2		

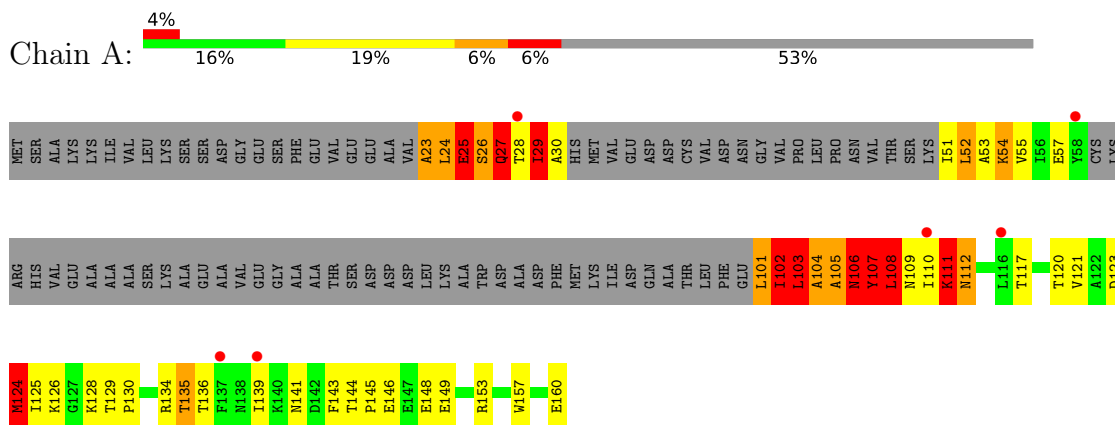
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	23	Total	O	0	0
			23	23		
5	B	203	Total	O	0	0
			203	203		

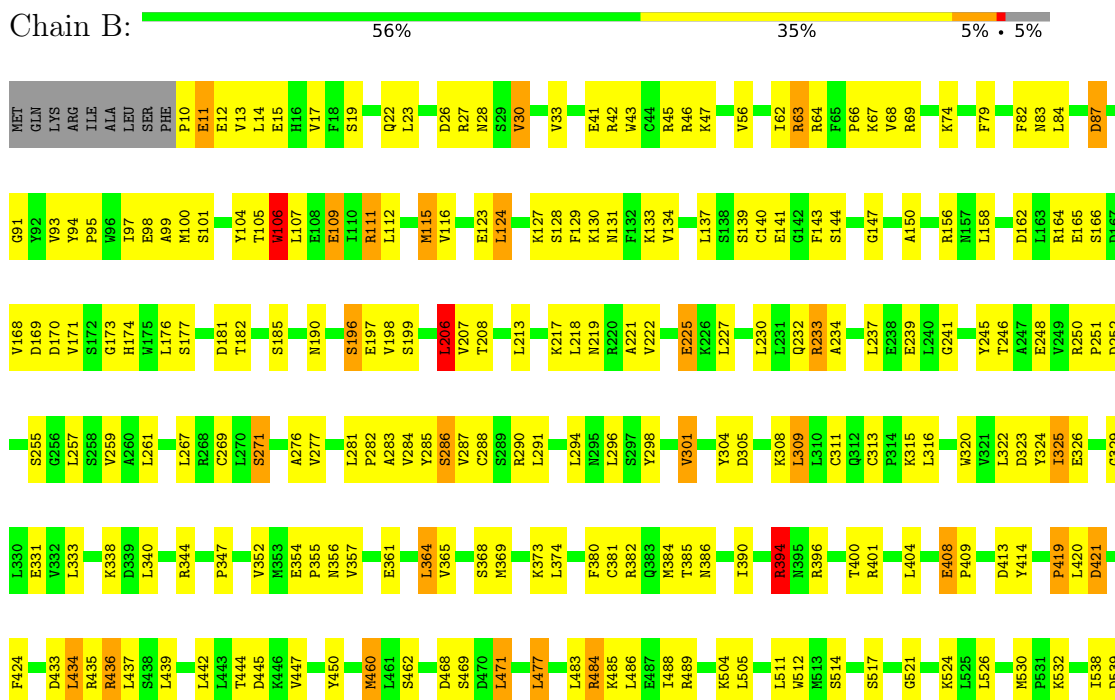
3 Residue-property plots

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: SKP1-like protein 1A



- Molecule 2: TRANSPORT INHIBITOR RESPONSE 1



E540	R541	P544	R547	P548	E549	P552	R555	R560	F572	N575	N576	ASP	GLN	ASP	ASP	SER	THR	MET	ARG	PHE	SER	SER	ARG	GLN	ILE	ILE	THR	THR	ASN	GLY	LEU
------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.26Å 80.84Å 124.75Å 90.00° 104.87° 90.00°	Depositor
Resolution (Å)	49.42 – 2.70 49.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	46.1 (49.42-2.70) 46.2 (49.42-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.272 0.201 , 0.281	Depositor DCC
R_{free} test set	1232 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5358	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 100.00 % 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 0.0000e+00. 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: IHP, 2S2

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	0.78	0/624	0.83	0/842
2	B	1.14	7/4558 (0.2%)	1.14	20/6178 (0.3%)
All	All	1.10	7/5182 (0.1%)	1.11	20/7020 (0.3%)

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	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	311	CYS	CB-SG	-9.10	1.66	1.82
2	B	225	GLU	CG-CD	5.81	1.60	1.51
2	B	408	GLU	CG-CD	5.63	1.60	1.51
2	B	381	CYS	CB-SG	-5.16	1.73	1.81
2	B	106	TRP	CE3-CZ3	5.13	1.47	1.38
2	B	196	SER	CB-OG	5.12	1.48	1.42
2	B	435	ARG	C-O	5.04	1.32	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	436	ARG	NE-CZ-NH2	11.66	126.13	120.30
2	B	436	ARG	NE-CZ-NH1	11.53	126.07	120.30
2	B	436	ARG	NH1-CZ-NH2	-10.70	107.62	119.40
2	B	436	ARG	CB-CA-C	-8.32	93.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	435	ARG	NE-CZ-NH2	-7.84	116.38	120.30
2	B	420	LEU	CB-CG-CD1	-7.15	98.84	111.00
2	B	404	LEU	CB-CG-CD2	-6.95	99.18	111.00
2	B	394	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	B	311	CYS	CA-CB-SG	-6.34	102.58	114.00
2	B	364	LEU	CB-CG-CD1	-6.25	100.37	111.00
2	B	526	LEU	CB-CG-CD2	-6.15	100.55	111.00
2	B	421	ASP	CB-CG-OD1	5.68	123.41	118.30
2	B	435	ARG	CA-C-O	5.53	131.70	120.10
2	B	477	LEU	CA-CB-CG	-5.35	102.99	115.30
2	B	484	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	B	488	ILE	CG1-CB-CG2	-5.20	99.96	111.40
2	B	486	LEU	N-CA-C	-5.17	97.03	111.00
2	B	206	LEU	CA-CB-CG	5.16	127.17	115.30
2	B	434	LEU	CA-CB-CG	-5.05	103.69	115.30
2	B	140	CYS	CA-CB-SG	-5.03	104.95	114.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ILE	Peptide
1	A	104	ALA	Peptide
1	A	106	ASN	Peptide
1	A	107	TYR	Peptide
1	A	108	LEU	Peptide
1	A	23	ALA	Peptide
1	A	27	GLN	Peptide
1	A	29	ILE	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	618	0	617	189	0
2	B	4461	0	4504	183	0
3	B	36	0	6	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	17	0	16	0	0
5	A	23	0	0	10	0
5	B	203	0	0	55	0
All	All	5358	0	5143	374	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 36.

All (374) 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:A:26:SER:CB	1:A:109:ASN:H	1.25	1.48
1:A:26:SER:HB2	1:A:109:ASN:N	1.24	1.40
1:A:23:ALA:CA	1:A:24:LEU:HD23	1.58	1.33
2:B:10:PRO:HD2	5:B:1050:HOH:O	1.28	1.27
1:A:108:LEU:C	1:A:108:LEU:HD12	1.52	1.25
1:A:23:ALA:C	1:A:24:LEU:HD23	1.57	1.23
1:A:29:ILE:CG2	1:A:30:ALA:HB2	1.68	1.22
1:A:102:ILE:N	1:A:103:LEU:HD12	1.55	1.21
2:B:419:PRO:HA	5:B:1203:HOH:O	1.37	1.20
1:A:29:ILE:HB	1:A:30:ALA:CB	1.70	1.20
2:B:277:VAL:HA	5:B:1199:HOH:O	1.40	1.18
2:B:281:LEU:O	2:B:284:VAL:HG22	1.45	1.17
1:A:26:SER:C	1:A:29:ILE:HD12	1.68	1.14
1:A:102:ILE:HD13	1:A:102:ILE:N	1.54	1.13
1:A:28:THR:HB	1:A:108:LEU:HA	1.26	1.11
2:B:74:LYS:NZ	3:B:1000:IHP:O26	1.84	1.10
1:A:29:ILE:HG22	1:A:30:ALA:N	1.54	1.10
1:A:29:ILE:CG2	1:A:30:ALA:CB	2.30	1.09
1:A:108:LEU:O	1:A:108:LEU:HD12	1.50	1.09
1:A:29:ILE:CB	1:A:30:ALA:HB3	1.82	1.08
1:A:29:ILE:CB	1:A:30:ALA:CB	2.32	1.08
1:A:26:SER:CA	1:A:29:ILE:HD12	1.85	1.05
1:A:110:ILE:HG22	1:A:110:ILE:O	1.56	1.02
2:B:352:VAL:HA	5:B:1046:HOH:O	1.58	1.02
2:B:170:ASP:OD1	2:B:196:SER:HB3	1.60	1.01
1:A:107:TYR:HB3	1:A:108:LEU:HG	1.43	1.01
1:A:101:LEU:N	1:A:103:LEU:HD13	1.78	0.99
2:B:442:LEU:HB3	5:B:1203:HOH:O	1.63	0.99
1:A:23:ALA:C	1:A:24:LEU:CD2	2.30	0.99
1:A:29:ILE:HG22	1:A:30:ALA:CA	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:SER:HA	1:A:109:ASN:HB3	1.45	0.98
1:A:108:LEU:CD1	1:A:108:LEU:C	2.30	0.98
1:A:102:ILE:H	1:A:103:LEU:CD1	1.76	0.97
1:A:26:SER:O	1:A:29:ILE:HD12	1.64	0.97
1:A:29:ILE:HB	1:A:30:ALA:HB3	0.96	0.96
1:A:101:LEU:HB2	1:A:102:ILE:HD13	1.46	0.95
1:A:29:ILE:HG21	1:A:30:ALA:HB2	1.47	0.95
1:A:26:SER:N	1:A:29:ILE:CD1	2.30	0.95
1:A:23:ALA:N	1:A:24:LEU:HD23	1.82	0.94
1:A:26:SER:CB	1:A:109:ASN:N	2.00	0.94
1:A:23:ALA:HB3	1:A:24:LEU:CD2	1.96	0.94
1:A:102:ILE:N	1:A:103:LEU:CD1	2.30	0.93
1:A:24:LEU:O	1:A:25:GLU:OE2	1.86	0.93
1:A:28:THR:O	1:A:29:ILE:HG13	1.69	0.93
1:A:102:ILE:N	1:A:102:ILE:CD1	2.30	0.92
1:A:26:SER:HB2	1:A:108:LEU:C	1.88	0.92
1:A:102:ILE:H	1:A:103:LEU:HD12	1.27	0.91
1:A:107:TYR:CD1	1:A:108:LEU:N	2.38	0.91
3:B:1000:IHP:O43	5:B:1160:HOH:O	1.87	0.91
1:A:26:SER:N	1:A:29:ILE:HD12	1.84	0.91
2:B:111:ARG:HH11	2:B:111:ARG:HG2	1.36	0.90
2:B:10:PRO:HD3	5:B:1068:HOH:O	1.70	0.89
1:A:23:ALA:CB	1:A:24:LEU:HD23	2.01	0.89
1:A:29:ILE:HG22	1:A:30:ALA:CB	1.98	0.88
1:A:124:MET:O	1:A:128:LYS:HE2	1.76	0.86
1:A:25:GLU:H	1:A:29:ILE:HD13	1.38	0.86
1:A:101:LEU:HB2	1:A:102:ILE:CD1	2.05	0.86
1:A:30:ALA:HB2	5:A:180:HOH:O	1.75	0.86
1:A:24:LEU:C	1:A:25:GLU:HG2	1.97	0.86
1:A:26:SER:CA	1:A:109:ASN:H	1.89	0.85
2:B:285:TYR:HA	2:B:288:CYS:SG	2.17	0.84
1:A:29:ILE:CG2	1:A:30:ALA:N	2.30	0.83
1:A:104:ALA:O	1:A:107:TYR:CB	2.26	0.83
1:A:102:ILE:O	1:A:104:ALA:CA	2.26	0.83
1:A:30:ALA:CB	5:A:180:HOH:O	2.25	0.83
1:A:102:ILE:O	1:A:104:ALA:HA	1.79	0.82
1:A:149:GLU:HB2	5:A:175:HOH:O	1.79	0.81
1:A:26:SER:CA	1:A:29:ILE:CD1	2.58	0.80
2:B:409:PRO:HA	5:B:1018:HOH:O	1.82	0.80
1:A:26:SER:HA	1:A:109:ASN:CB	2.10	0.79
1:A:28:THR:CB	1:A:108:LEU:HA	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:HG22	1:A:30:ALA:HB2	1.57	0.79
1:A:23:ALA:O	1:A:24:LEU:CD2	2.30	0.79
1:A:26:SER:O	1:A:29:ILE:CD1	2.30	0.79
1:A:26:SER:HB2	1:A:108:LEU:CA	2.12	0.79
1:A:101:LEU:C	1:A:102:ILE:HD13	2.02	0.79
1:A:24:LEU:HG	1:A:24:LEU:O	1.80	0.79
2:B:176:LEU:HD21	2:B:206:LEU:HD12	1.65	0.78
2:B:352:VAL:O	2:B:382:ARG:NH2	2.17	0.78
1:A:107:TYR:HB3	1:A:108:LEU:CG	2.14	0.78
1:A:23:ALA:CB	1:A:24:LEU:CD2	2.60	0.77
1:A:108:LEU:CD1	1:A:108:LEU:O	2.30	0.77
1:A:146:GLU:HG2	5:A:170:HOH:O	1.85	0.77
1:A:110:ILE:O	1:A:110:ILE:CG2	2.30	0.76
2:B:30:VAL:HG22	2:B:41:GLU:HG3	1.68	0.76
1:A:24:LEU:O	1:A:25:GLU:HG2	1.85	0.75
1:A:101:LEU:N	1:A:103:LEU:CD1	2.49	0.75
1:A:26:SER:O	1:A:29:ILE:CG1	2.35	0.75
1:A:26:SER:OG	1:A:29:ILE:HG13	1.87	0.74
1:A:26:SER:OG	1:A:29:ILE:CD1	2.34	0.74
2:B:282:PRO:HA	2:B:285:TYR:CZ	2.23	0.74
2:B:287:VAL:HG12	2:B:291:LEU:HD13	1.69	0.74
1:A:108:LEU:HD12	1:A:109:ASN:N	2.02	0.74
1:A:129:THR:HB	1:A:130:PRO:HD2	1.71	0.73
1:A:23:ALA:CA	1:A:24:LEU:CD2	2.53	0.73
2:B:489:ARG:HD3	5:B:1092:HOH:O	1.89	0.72
1:A:105:ALA:O	1:A:108:LEU:O	2.08	0.72
1:A:29:ILE:HG22	1:A:30:ALA:H	1.53	0.72
1:A:104:ALA:CB	1:A:107:TYR:HB2	2.19	0.72
1:A:26:SER:HB3	1:A:109:ASN:H	1.48	0.72
1:A:24:LEU:O	1:A:25:GLU:CG	2.38	0.72
2:B:109:GLU:HB3	2:B:134:VAL:HB	1.72	0.71
1:A:26:SER:C	1:A:28:THR:N	2.40	0.71
1:A:54:LYS:HA	1:A:57:GLU:HG2	1.69	0.71
1:A:26:SER:HB2	1:A:108:LEU:HA	1.71	0.71
2:B:436:ARG:HG3	2:B:437:LEU:N	2.05	0.71
1:A:28:THR:HG21	1:A:108:LEU:H	1.53	0.71
1:A:26:SER:O	1:A:28:THR:C	2.30	0.70
1:A:23:ALA:O	1:A:24:LEU:HD22	1.90	0.70
2:B:505:LEU:HD23	2:B:505:LEU:N	2.06	0.70
1:A:102:ILE:HD13	1:A:102:ILE:H	1.55	0.70
2:B:331:GLU:HG2	5:B:1125:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:CB	5:A:175:HOH:O	2.34	0.70
2:B:394:ARG:HH11	2:B:394:ARG:HG2	1.55	0.70
2:B:401:ARG:NH1	3:B:1000:IHP:O23	2.25	0.69
2:B:352:VAL:HG12	2:B:354:GLU:H	1.57	0.69
2:B:174:HIS:HB3	5:B:1043:HOH:O	1.92	0.69
2:B:333:LEU:HD21	2:B:340:LEU:HD22	1.74	0.69
2:B:10:PRO:CB	5:B:1088:HOH:O	2.39	0.68
2:B:539:ASP:OD2	2:B:541:ARG:HD2	1.92	0.68
1:A:104:ALA:HB1	1:A:107:TYR:HB2	1.75	0.68
1:A:104:ALA:O	1:A:107:TYR:HB2	1.91	0.68
2:B:100:MET:HG2	2:B:104:TYR:CD1	2.28	0.68
1:A:26:SER:CB	1:A:29:ILE:CD1	2.71	0.68
1:A:124:MET:CE	1:A:124:MET:HA	2.23	0.67
2:B:30:VAL:CG2	2:B:41:GLU:HG3	2.24	0.67
2:B:143:PHE:CE1	2:B:168:VAL:HG22	2.30	0.67
2:B:433:ASP:HB3	5:B:1052:HOH:O	1.95	0.67
1:A:107:TYR:HD1	1:A:107:TYR:C	1.97	0.67
1:A:26:SER:CB	1:A:29:ILE:HD11	2.24	0.67
2:B:286:SER:HA	5:B:1025:HOH:O	1.93	0.67
1:A:107:TYR:CD1	1:A:107:TYR:C	2.67	0.67
1:A:110:ILE:O	1:A:111:LYS:C	2.34	0.66
2:B:552:PRO:HB3	5:B:1104:HOH:O	1.95	0.66
1:A:107:TYR:HD1	1:A:108:LEU:N	1.94	0.66
2:B:301:VAL:HG13	2:B:305:ASP:HB2	1.76	0.65
1:A:26:SER:O	1:A:28:THR:N	2.30	0.65
1:A:134:ARG:HB2	1:A:139:ILE:O	1.97	0.65
1:A:102:ILE:H	1:A:103:LEU:HD11	1.62	0.65
1:A:25:GLU:O	1:A:27:GLN:N	2.30	0.65
2:B:46:ARG:HD3	5:B:1172:HOH:O	1.96	0.65
2:B:106:TRP:C	5:B:1117:HOH:O	2.35	0.65
2:B:111:ARG:HH11	2:B:111:ARG:CG	2.08	0.64
1:A:107:TYR:N	1:A:108:LEU:O	2.30	0.64
1:A:23:ALA:N	1:A:24:LEU:O	2.30	0.64
2:B:63:ARG:HD2	5:B:1161:HOH:O	1.96	0.64
2:B:442:LEU:CG	5:B:1203:HOH:O	2.45	0.64
1:A:102:ILE:O	1:A:104:ALA:N	2.30	0.64
1:A:103:LEU:HA	1:A:104:ALA:HB2	1.80	0.64
2:B:368:SER:HB2	2:B:396:ARG:HG3	1.79	0.64
1:A:104:ALA:O	1:A:108:LEU:HG	1.98	0.63
2:B:447:VAL:O	2:B:450:TYR:HB2	1.98	0.63
1:A:121:VAL:O	1:A:124:MET:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ALA:O	1:A:107:TYR:N	2.29	0.63
1:A:146:GLU:HB2	5:A:174:HOH:O	1.98	0.62
2:B:97:ILE:HG22	2:B:124:LEU:HD13	1.81	0.62
2:B:408:GLU:HB3	5:B:1030:HOH:O	1.98	0.62
1:A:23:ALA:N	1:A:24:LEU:CD2	2.59	0.62
1:A:26:SER:OG	1:A:29:ILE:CG1	2.47	0.62
2:B:255:SER:O	2:B:259:VAL:HG23	1.99	0.62
2:B:285:TYR:N	5:B:1132:HOH:O	2.31	0.62
2:B:460:MET:HE3	5:B:1005:HOH:O	1.98	0.62
1:A:102:ILE:CA	1:A:103:LEU:HD12	2.28	0.62
2:B:11:GLU:CB	5:B:1151:HOH:O	2.48	0.62
1:A:160:GLU:HG3	2:B:28:ASN:ND2	2.15	0.62
1:A:26:SER:CB	1:A:108:LEU:HA	2.30	0.61
2:B:384:MET:HG3	2:B:385:THR:N	2.13	0.61
1:A:23:ALA:HB3	1:A:24:LEU:HD21	1.80	0.61
1:A:143:PHE:HB3	1:A:148:GLU:HB2	1.82	0.61
1:A:28:THR:C	1:A:29:ILE:HG13	2.20	0.61
2:B:27:ARG:HB3	2:B:45:ARG:NH2	2.15	0.61
1:A:107:TYR:HB3	1:A:108:LEU:CB	2.31	0.61
2:B:97:ILE:O	2:B:101:SER:N	2.31	0.61
2:B:333:LEU:HD21	2:B:340:LEU:CD2	2.29	0.60
2:B:94:TYR:HB3	2:B:95:PRO:HD3	1.83	0.60
2:B:322:LEU:O	2:B:325:ILE:HG22	2.01	0.60
1:A:105:ALA:O	1:A:107:TYR:N	2.34	0.60
1:A:104:ALA:O	1:A:107:TYR:HB3	2.00	0.60
2:B:445:ASP:OD2	2:B:468:ASP:N	2.25	0.60
1:A:125:ILE:O	1:A:126:LYS:C	2.39	0.60
1:A:51:ILE:C	1:A:53:ALA:H	2.06	0.60
1:A:103:LEU:N	1:A:103:LEU:HD12	2.18	0.59
2:B:197:GLU:HG3	2:B:221:ALA:HB1	1.83	0.59
1:A:105:ALA:O	1:A:106:ASN:C	2.41	0.59
2:B:91:GLY:O	2:B:115:MET:HE3	2.01	0.59
1:A:24:LEU:O	1:A:25:GLU:CD	2.40	0.59
2:B:539:ASP:O	2:B:572:PHE:HB2	2.03	0.59
2:B:442:LEU:CB	5:B:1203:HOH:O	2.34	0.58
2:B:208:THR:HA	5:B:1100:HOH:O	2.02	0.58
2:B:93:VAL:HG12	2:B:116:VAL:O	2.03	0.58
1:A:26:SER:CB	1:A:108:LEU:CA	2.82	0.58
2:B:144:SER:HB3	2:B:169:ASP:HB3	1.85	0.58
1:A:141:ASN:OD1	1:A:143:PHE:N	2.32	0.58
1:A:107:TYR:CG	1:A:108:LEU:N	2.70	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:ILE:O	2:B:329:GLY:HA3	2.04	0.57
2:B:111:ARG:NH1	2:B:111:ARG:HG2	2.15	0.57
1:A:26:SER:HA	1:A:109:ASN:CA	2.35	0.57
1:A:24:LEU:C	1:A:25:GLU:CG	2.72	0.57
2:B:47:LYS:HE3	5:B:1167:HOH:O	2.05	0.57
1:A:124:MET:HE2	1:A:124:MET:HA	1.87	0.57
1:A:26:SER:O	1:A:29:ILE:CB	2.53	0.57
2:B:12:GLU:HA	5:B:1147:HOH:O	2.05	0.57
2:B:87:ASP:N	2:B:87:ASP:OD2	2.37	0.57
1:A:101:LEU:CB	1:A:102:ILE:HD13	2.28	0.56
2:B:521:GLY:HA3	5:B:1066:HOH:O	2.03	0.56
1:A:160:GLU:C	5:A:185:HOH:O	2.43	0.56
1:A:26:SER:O	1:A:29:ILE:N	2.38	0.56
2:B:107:LEU:HB3	2:B:129:PHE:CD2	2.40	0.56
2:B:185:SER:HA	5:B:1093:HOH:O	2.05	0.56
1:A:126:LYS:HD3	5:B:1128:HOH:O	2.05	0.56
2:B:144:SER:CB	2:B:169:ASP:HB3	2.36	0.56
2:B:401:ARG:HG2	2:B:436:ARG:HB3	1.87	0.56
2:B:82:PHE:O	2:B:83:ASN:HB2	2.05	0.56
2:B:294:LEU:HD21	2:B:296:LEU:HD11	1.87	0.55
1:A:24:LEU:HB2	5:A:180:HOH:O	2.07	0.55
2:B:261:LEU:CD1	2:B:284:VAL:HG12	2.37	0.55
2:B:112:LEU:HB3	2:B:115:MET:HG3	1.89	0.54
2:B:207:VAL:HG21	2:B:230:LEU:HD22	1.89	0.54
2:B:394:ARG:CG	2:B:394:ARG:HH11	2.21	0.54
1:A:26:SER:OG	1:A:29:ILE:HD11	2.06	0.54
2:B:10:PRO:HB2	5:B:1088:HOH:O	2.04	0.54
2:B:538:ILE:O	2:B:555:ARG:HB2	2.07	0.54
2:B:11:GLU:HB2	5:B:1151:HOH:O	2.07	0.54
2:B:30:VAL:O	2:B:33:VAL:HG13	2.08	0.54
1:A:26:SER:HB3	1:A:108:LEU:HD13	1.90	0.53
2:B:91:GLY:O	2:B:115:MET:CE	2.55	0.53
2:B:544:PRO:HA	2:B:547:ARG:NH2	2.23	0.53
2:B:137:LEU:O	2:B:166:SER:OG	2.27	0.53
2:B:361:GLU:O	2:B:365:VAL:HG23	2.08	0.53
1:A:102:ILE:O	1:A:105:ALA:HB3	2.09	0.53
2:B:250:ARG:HB3	2:B:252:ASP:OD2	2.10	0.52
2:B:131:ASN:HB2	5:B:1117:HOH:O	2.09	0.52
2:B:47:LYS:CE	5:B:1167:HOH:O	2.57	0.52
2:B:287:VAL:CG1	2:B:291:LEU:HD13	2.39	0.52
2:B:79:PHE:CD2	2:B:84:LEU:HD12	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ALA:C	1:A:107:TYR:H	2.13	0.52
1:A:26:SER:CA	1:A:109:ASN:HB3	2.29	0.51
2:B:575:ASN:C	2:B:575:ASN:HD22	2.13	0.51
2:B:232:GLN:HG3	5:B:1169:HOH:O	2.10	0.51
2:B:27:ARG:HD3	2:B:41:GLU:OE2	2.11	0.51
2:B:436:ARG:HD3	5:B:1160:HOH:O	2.09	0.51
1:A:105:ALA:C	1:A:107:TYR:N	2.64	0.51
1:A:28:THR:HB	1:A:108:LEU:CA	2.19	0.51
1:A:26:SER:OG	1:A:28:THR:HB	2.11	0.51
2:B:239:GLU:HG2	2:B:269:CYS:HB2	1.94	0.50
2:B:524:LYS:HE2	2:B:549:GLU:OE2	2.11	0.50
3:B:1000:IHP:O25	3:B:1000:IHP:O16	2.30	0.50
2:B:400:THR:O	2:B:401:ARG:HG3	2.12	0.50
2:B:97:ILE:O	2:B:101:SER:HB3	2.12	0.50
3:B:1000:IHP:O44	3:B:1000:IHP:O33	2.30	0.50
2:B:442:LEU:HG	5:B:1203:HOH:O	2.09	0.50
2:B:43:TRP:HE3	2:B:67:LYS:HD2	1.75	0.50
2:B:309:LEU:HD23	2:B:309:LEU:O	2.11	0.50
1:A:109:ASN:OD1	1:A:109:ASN:O	2.30	0.50
2:B:171:VAL:CG1	5:B:1119:HOH:O	2.59	0.49
1:A:24:LEU:CG	1:A:24:LEU:O	2.58	0.49
3:B:1000:IHP:O13	3:B:1000:IHP:O32	2.30	0.49
2:B:282:PRO:HA	2:B:285:TYR:CE1	2.47	0.49
1:A:26:SER:OG	1:A:28:THR:O	2.30	0.49
1:A:53:ALA:C	1:A:55:VAL:H	2.15	0.49
2:B:277:VAL:HG22	5:B:1199:HOH:O	2.13	0.49
2:B:386:ASN:O	2:B:390:ILE:HG13	2.12	0.49
2:B:62:ILE:CD1	2:B:99:ALA:HB1	2.42	0.49
2:B:124:LEU:HD22	2:B:128:SER:OG	2.12	0.49
1:A:26:SER:O	1:A:26:SER:OG	2.30	0.48
2:B:105:THR:HB	5:B:1090:HOH:O	2.13	0.48
2:B:261:LEU:HD13	2:B:284:VAL:HG12	1.95	0.48
2:B:552:PRO:HA	5:B:1104:HOH:O	2.14	0.48
1:A:28:THR:HG21	1:A:108:LEU:N	2.26	0.48
2:B:245:TYR:O	2:B:276:ALA:HA	2.14	0.48
1:A:23:ALA:N	1:A:25:GLU:CD	2.68	0.48
2:B:517:SER:C	5:B:1104:HOH:O	2.51	0.48
2:B:79:PHE:HD2	2:B:84:LEU:HD12	1.79	0.48
2:B:111:ARG:NH1	2:B:111:ARG:CG	2.71	0.47
1:A:108:LEU:CD1	1:A:110:ILE:HG13	2.44	0.47
1:A:101:LEU:HB2	1:A:102:ILE:HD11	1.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:THR:HG22	1:A:28:THR:O	2.14	0.47
1:A:124:MET:O	1:A:128:LYS:CE	2.56	0.47
2:B:484:ARG:NH2	2:B:485:LYS:HE2	2.30	0.47
2:B:219:ASN:HB2	5:B:1133:HOH:O	2.13	0.47
1:A:26:SER:HA	1:A:109:ASN:N	2.30	0.47
1:A:26:SER:O	1:A:29:ILE:HB	2.14	0.47
2:B:512:TRP:C	2:B:512:TRP:CD1	2.88	0.47
2:B:225:GLU:HB2	5:B:1174:HOH:O	2.15	0.47
1:A:26:SER:C	1:A:28:THR:H	2.18	0.46
2:B:281:LEU:N	2:B:282:PRO:CD	2.78	0.46
2:B:514:SER:HB3	2:B:555:ARG:HG2	1.96	0.46
2:B:100:MET:HG2	2:B:104:TYR:HD1	1.79	0.46
2:B:177:SER:HA	5:B:1183:HOH:O	2.15	0.46
1:A:29:ILE:CB	1:A:30:ALA:HB2	2.17	0.46
1:A:26:SER:N	1:A:29:ILE:HD11	2.25	0.46
1:A:26:SER:HA	1:A:109:ASN:H	1.77	0.46
2:B:282:PRO:HA	2:B:285:TYR:CE2	2.50	0.46
2:B:373:LYS:HB2	5:B:1051:HOH:O	2.16	0.46
2:B:271:SER:HB2	5:B:1162:HOH:O	2.16	0.46
1:A:101:LEU:HD13	5:A:182:HOH:O	2.15	0.45
2:B:130:LYS:N	5:B:1035:HOH:O	2.48	0.45
2:B:460:MET:CE	2:B:485:LYS:HZ2	2.29	0.45
1:A:135:THR:HG22	1:A:136:THR:N	2.32	0.45
2:B:304:TYR:CE2	2:B:308:LYS:HD3	2.52	0.45
1:A:104:ALA:HB3	1:A:107:TYR:HB2	1.95	0.45
2:B:190:ASN:HA	2:B:217:LYS:HB2	1.99	0.45
1:A:141:ASN:OD1	1:A:143:PHE:HB2	2.17	0.45
2:B:434:LEU:HD12	2:B:434:LEU:HA	1.58	0.45
2:B:43:TRP:CZ3	2:B:66:PRO:HG2	2.51	0.45
2:B:10:PRO:C	5:B:1088:HOH:O	2.55	0.45
2:B:324:TYR:O	2:B:326:GLU:HG3	2.17	0.45
1:A:153:ARG:NH1	2:B:532:LYS:HE2	2.32	0.45
1:A:26:SER:CA	1:A:109:ASN:N	2.65	0.44
2:B:356:ASN:OD1	2:B:357:VAL:HG13	2.18	0.44
2:B:287:VAL:HG12	2:B:291:LEU:CD1	2.43	0.44
2:B:320:TRP:CE2	2:B:344:ARG:HD2	2.52	0.44
2:B:419:PRO:CA	5:B:1203:HOH:O	2.20	0.44
2:B:162:ASP:HA	2:B:190:ASN:HB3	2.00	0.44
1:A:102:ILE:O	1:A:105:ALA:N	2.51	0.43
1:A:123:ASP:C	1:A:125:ILE:N	2.72	0.43
2:B:42:ARG:HB2	2:B:64:ARG:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:GLY:O	2:B:150:ALA:HB3	2.18	0.43
2:B:460:MET:CE	2:B:485:LYS:NZ	2.81	0.43
1:A:102:ILE:HG23	1:A:117:THR:OG1	2.17	0.43
1:A:157:TRP:CE2	2:B:560:ARG:HD2	2.53	0.43
2:B:288:CYS:O	2:B:313:CYS:HA	2.19	0.43
2:B:352:VAL:CG1	2:B:354:GLU:HB2	2.48	0.43
2:B:385:THR:CG2	2:B:414:TYR:CE2	3.01	0.43
2:B:66:PRO:HB3	5:B:1047:HOH:O	2.18	0.43
2:B:477:LEU:O	2:B:504:LYS:HD3	2.18	0.43
2:B:233:ARG:NH1	5:B:1054:HOH:O	2.51	0.43
1:A:144:THR:O	1:A:146:GLU:N	2.51	0.43
2:B:352:VAL:C	2:B:382:ARG:HH21	2.23	0.43
1:A:110:ILE:O	1:A:112:ASN:N	2.51	0.42
2:B:94:TYR:CE2	2:B:98:GLU:OE1	2.72	0.42
2:B:115:MET:HB3	2:B:115:MET:HE2	1.64	0.42
2:B:100:MET:HG2	2:B:104:TYR:CE1	2.54	0.42
2:B:552:PRO:CA	5:B:1104:HOH:O	2.67	0.42
1:A:28:THR:CB	1:A:108:LEU:CA	2.88	0.42
2:B:380:PHE:N	2:B:380:PHE:CD1	2.88	0.42
2:B:413:ASP:C	2:B:413:ASP:OD1	2.57	0.42
2:B:287:VAL:H	2:B:287:VAL:HG23	1.51	0.42
3:B:1000:IHP:O14	3:B:1000:IHP:O33	2.38	0.42
2:B:171:VAL:HG11	5:B:1119:HOH:O	2.19	0.42
2:B:246:THR:HA	2:B:277:VAL:HG23	2.01	0.42
2:B:315:LYS:HG2	5:B:1198:HOH:O	2.20	0.42
2:B:385:THR:CG2	2:B:414:TYR:HE2	2.33	0.42
2:B:218:LEU:HD13	2:B:222:VAL:HG11	2.01	0.42
2:B:257:LEU:HA	2:B:257:LEU:HD23	1.70	0.41
2:B:26:ASP:O	2:B:30:VAL:HG13	2.19	0.41
1:A:101:LEU:HD12	1:A:103:LEU:HD11	2.01	0.41
1:A:144:THR:C	5:A:170:HOH:O	2.59	0.41
2:B:325:ILE:O	2:B:325:ILE:HG13	2.18	0.41
2:B:316:LEU:HA	2:B:316:LEU:HD12	1.75	0.41
1:A:25:GLU:O	1:A:26:SER:C	2.59	0.41
2:B:14:LEU:O	2:B:15:GLU:C	2.59	0.41
2:B:207:VAL:CG1	2:B:234:ALA:HB2	2.51	0.41
1:A:108:LEU:O	1:A:108:LEU:CG	2.67	0.41
1:A:26:SER:O	1:A:29:ILE:HG13	2.17	0.41
1:A:25:GLU:C	1:A:29:ILE:HD12	2.38	0.41
2:B:19:SER:O	2:B:22:GLN:NE2	2.50	0.41
2:B:251:PRO:O	2:B:255:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:471:LEU:HA	2:B:471:LEU:HD23	1.87	0.41
2:B:469:SER:C	2:B:471:LEU:N	2.74	0.41
2:B:444:THR:HB	2:B:468:ASP:OD2	2.20	0.41
1:A:107:TYR:CG	1:A:108:LEU:HB3	2.54	0.41
2:B:469:SER:OG	2:B:471:LEU:HB2	2.21	0.41
1:A:102:ILE:C	1:A:103:LEU:HD12	2.41	0.41
1:A:106:ASN:O	1:A:107:TYR:O	2.39	0.41
2:B:133:LYS:O	2:B:158:LEU:HD12	2.19	0.41
2:B:13:VAL:O	2:B:17:VAL:HG23	2.21	0.41
2:B:323:ASP:OD2	2:B:347:PRO:HA	2.21	0.41
1:A:129:THR:HB	1:A:130:PRO:CD	2.46	0.41
2:B:445:ASP:CG	2:B:468:ASP:HB2	2.41	0.40
1:A:54:LYS:HA	1:A:57:GLU:CG	2.46	0.40
1:A:124:MET:HE3	1:A:124:MET:HA	2.03	0.40
2:B:241:GLY:HA2	2:B:271:SER:O	2.22	0.40
2:B:424:PHE:CE2	2:B:439:LEU:HD23	2.57	0.40

There are no symmetry-related clashes.

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	70/160 (44%)	40 (57%)	15 (21%)	15 (21%)	0	0
2	B	565/594 (95%)	508 (90%)	50 (9%)	7 (1%)	13	32
All	All	635/754 (84%)	548 (86%)	65 (10%)	22 (4%)	3	8

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	27	GLN

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Mol	Chain	Res	Type
1	A	29	ILE
1	A	103	LEU
1	A	105	ALA
1	A	107	TYR
1	A	108	LEU
2	B	11	GLU
1	A	52	LEU
1	A	106	ASN
1	A	124	MET
1	A	145	PRO
2	B	181	ASP
1	A	24	LEU
1	A	25	GLU
1	A	135	THR
2	B	106	TRP
2	B	283	ALA
2	B	355	PRO
1	A	111	LYS
2	B	56	VAL
2	B	173	GLY

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	68/137 (50%)	56 (82%)	12 (18%)	2	4
2	B	500/525 (95%)	451 (90%)	49 (10%)	8	18
All	All	568/662 (86%)	507 (89%)	61 (11%)	6	15

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	52	LEU
1	A	54	LYS

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Mol	Chain	Res	Type
1	A	101	LEU
1	A	102	ILE
1	A	103	LEU
1	A	107	TYR
1	A	108	LEU
1	A	111	LYS
1	A	112	ASN
1	A	120	THR
1	A	124	MET
2	B	23	LEU
2	B	30	VAL
2	B	63	ARG
2	B	68	VAL
2	B	69	ARG
2	B	87	ASP
2	B	109	GLU
2	B	111	ARG
2	B	115	MET
2	B	123	GLU
2	B	124	LEU
2	B	127	LYS
2	B	139	SER
2	B	141	GLU
2	B	156	ARG
2	B	164	ARG
2	B	165	GLU
2	B	182	THR
2	B	198	VAL
2	B	199	SER
2	B	206	LEU
2	B	213	LEU
2	B	227	LEU
2	B	233	ARG
2	B	237	LEU
2	B	248	GLU
2	B	267	LEU
2	B	271	SER
2	B	286	SER
2	B	290	ARG
2	B	298	TYR
2	B	301	VAL
2	B	309	LEU

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Mol	Chain	Res	Type
2	B	325	ILE
2	B	338	LYS
2	B	364	LEU
2	B	369	MET
2	B	374	LEU
2	B	394	ARG
2	B	419	PRO
2	B	421	ASP
2	B	460	MET
2	B	462	SER
2	B	471	LEU
2	B	483	LEU
2	B	511	LEU
2	B	530	MET
2	B	541	ARG
2	B	575	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
2	B	178	HIS
2	B	383	GLN
2	B	501	ASN
2	B	575	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	2S2	B	1001	-	15,18,18	1.84	3 (20%)	16,24,24	4.37	4 (25%)
3	IHP	B	1000	-	36,36,36	0.90	1 (2%)	54,60,60	0.72	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	2S2	B	1001	-	-	3/5/12/12	0/2/2/2
3	IHP	B	1000	-	-	9/30/54/54	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	2S2	CAH-NM	-5.14	1.26	1.36
4	B	1001	2S2	CAH-CAO	-3.16	1.28	1.37
3	B	1000	IHP	P6-O16	-2.44	1.54	1.59
4	B	1001	2S2	CAO-CAR	-2.32	1.50	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1001	2S2	CAO-CAH-NM	16.12	139.55	108.79
4	B	1001	2S2	CAN-CAR-CAO	-3.45	106.15	111.17
4	B	1001	2S2	CAG-CAQ-CAP	3.28	122.51	118.17
4	B	1001	2S2	CAF-CAP-CAQ	-2.51	116.17	120.76

There are no chirality outliers.

All (12) torsion outliers are listed below:

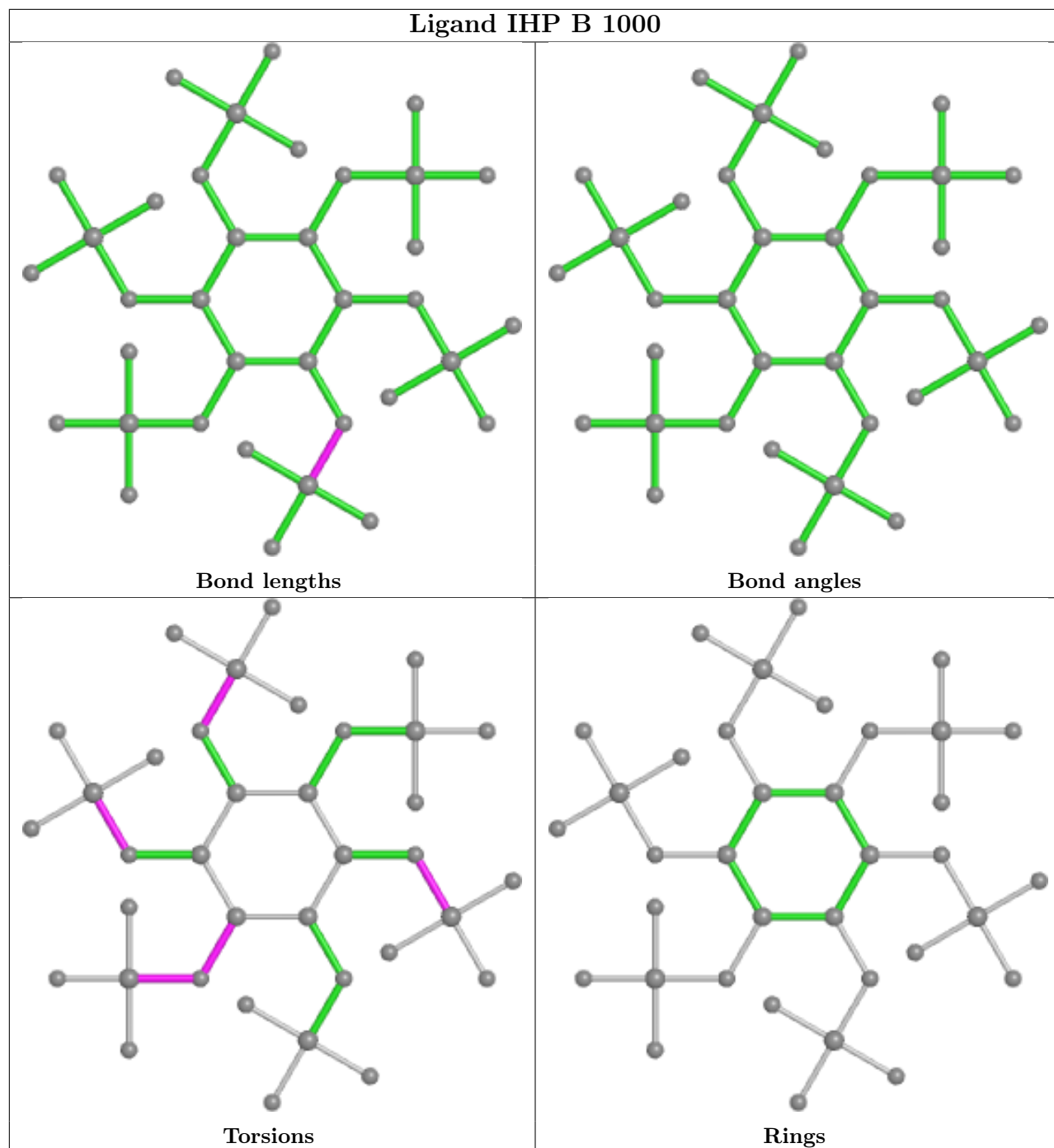
Mol	Chain	Res	Type	Atoms
3	B	1000	IHP	C1-O11-P1-O21
3	B	1000	IHP	C1-O11-P1-O41
3	B	1000	IHP	C3-O13-P3-O23
4	B	1001	2S2	CAK-CAL-CAR-CAO
4	B	1001	2S2	CAK-CAL-CAR-CAN
4	B	1001	2S2	CAJ-CAK-CAL-CAR
3	B	1000	IHP	C2-O12-P2-O22
3	B	1000	IHP	C3-O13-P3-O33
3	B	1000	IHP	C5-O15-P5-O35
3	B	1000	IHP	C2-C1-O11-P1
3	B	1000	IHP	C2-O12-P2-O32
3	B	1000	IHP	C3-O13-P3-O43

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	IHP	7	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	76/160 (47%)	0.41	6 (7%) 12 10	30, 60, 71, 72	0
2	B	567/594 (95%)	-0.55	0 100 100	20, 35, 50, 67	0
All	All	643/754 (85%)	-0.44	6 (0%) 84 85	20, 36, 64, 72	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	LEU	3.3
1	A	137	PHE	2.7
1	A	58	TYR	2.6
1	A	139	ILE	2.3
1	A	110	ILE	2.1
1	A	28	THR	2.1

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

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

6.3 Carbohydrates [i](#)

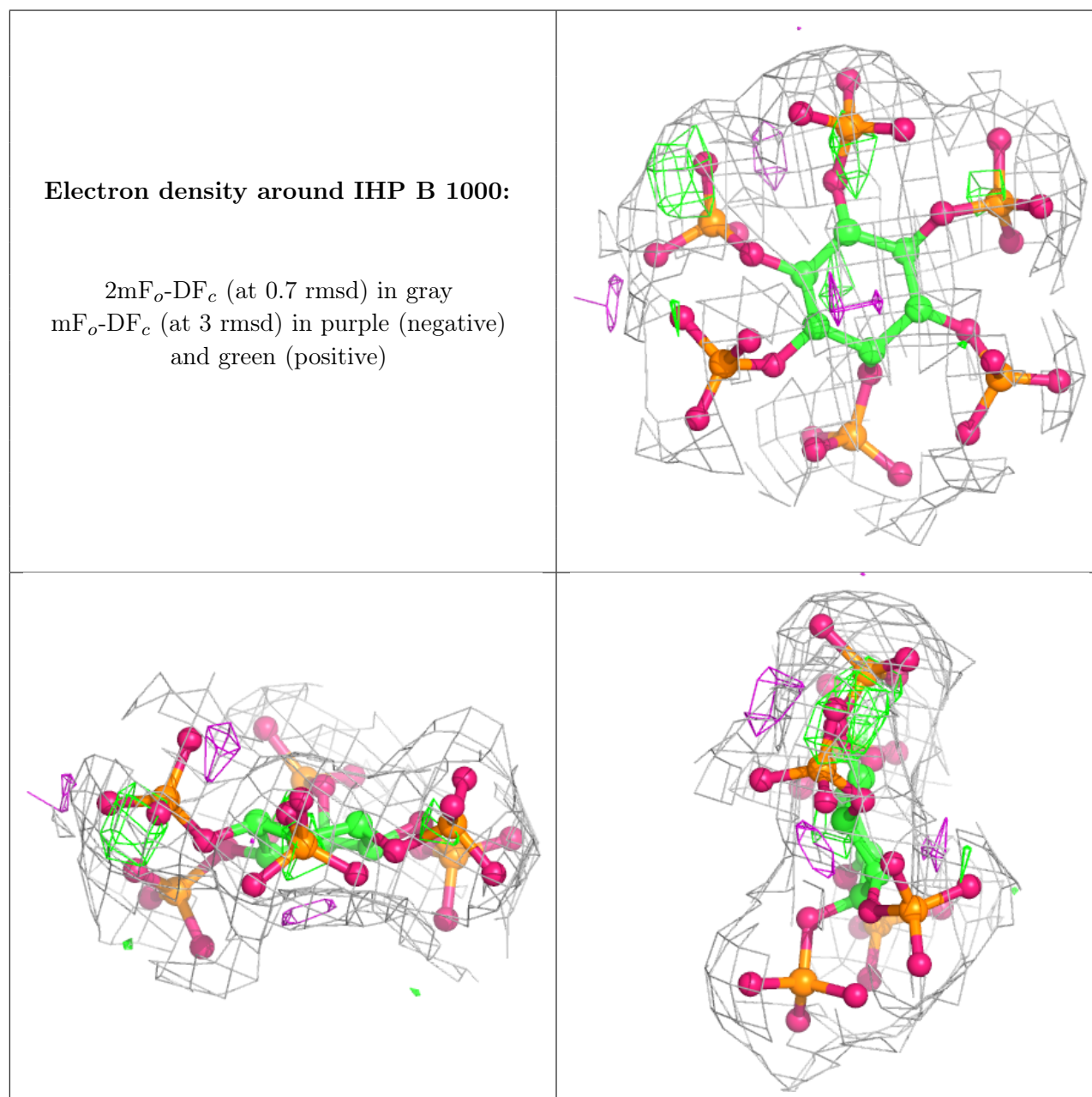
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
3	IHP	B	1000	36/36	0.96	0.27	60,75,98,100	0
4	2S2	B	1001	17/17	0.97	0.27	82,89,92,93	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.