



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:47 AM GMT

PDB ID : 3C6P  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

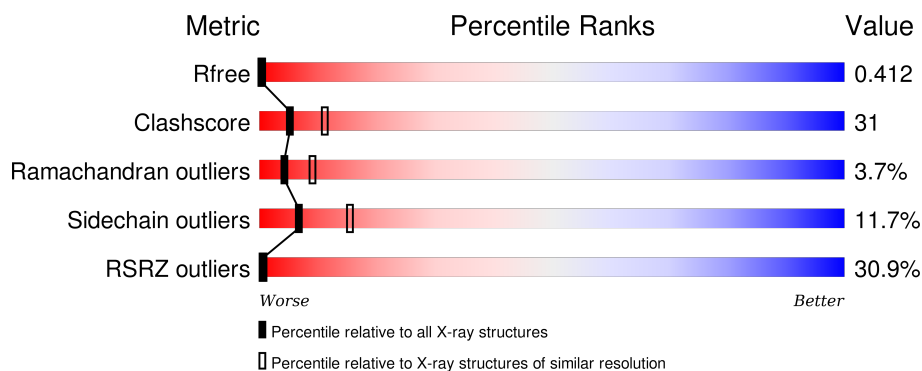
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

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
4	2S3	B	1001	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5535 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.

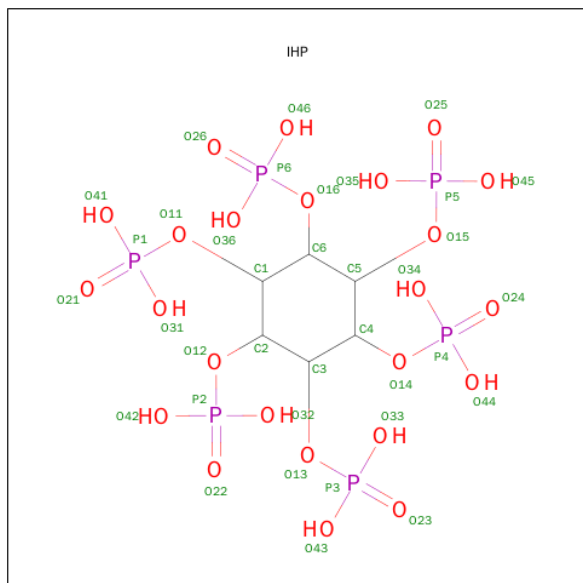
- Molecule 1 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			721	459	117	143	2			

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

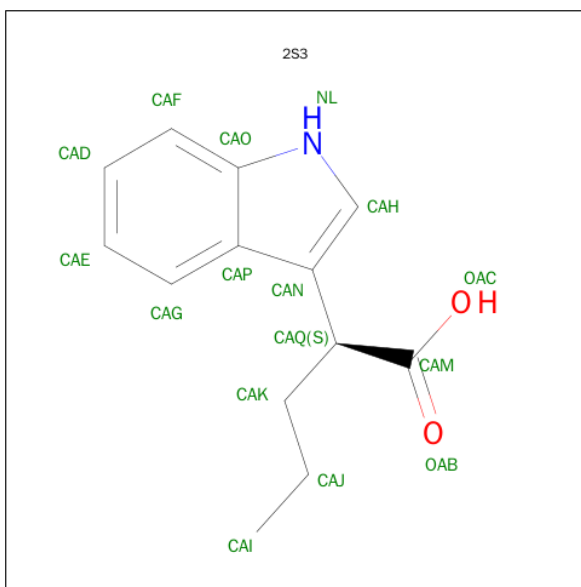
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	567	Total	C	N	O	S	0	0	0
			4461	2850	754	820	37			

- 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)PENTANOIC ACID (three-letter code: 2S3) (formula:  $C_{13}H_{15}NO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			16	13	1	2		

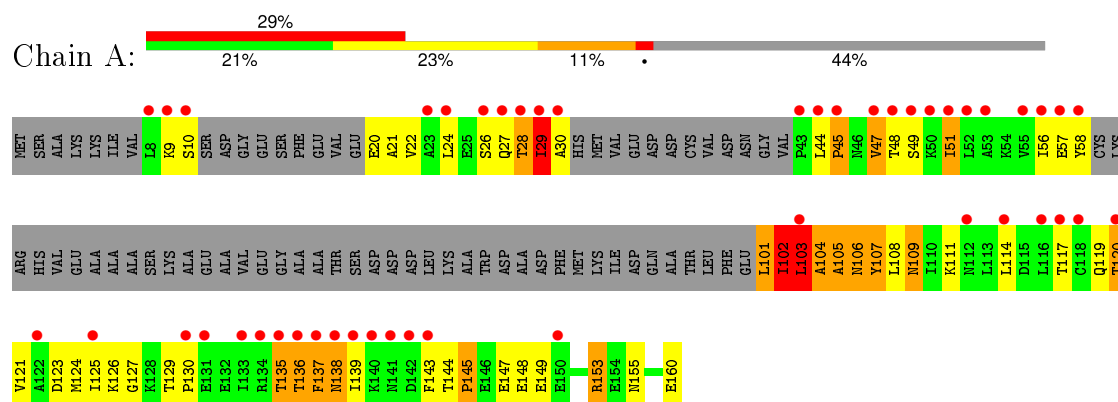
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		
5	B	264	Total	O	0	0
			264	264		

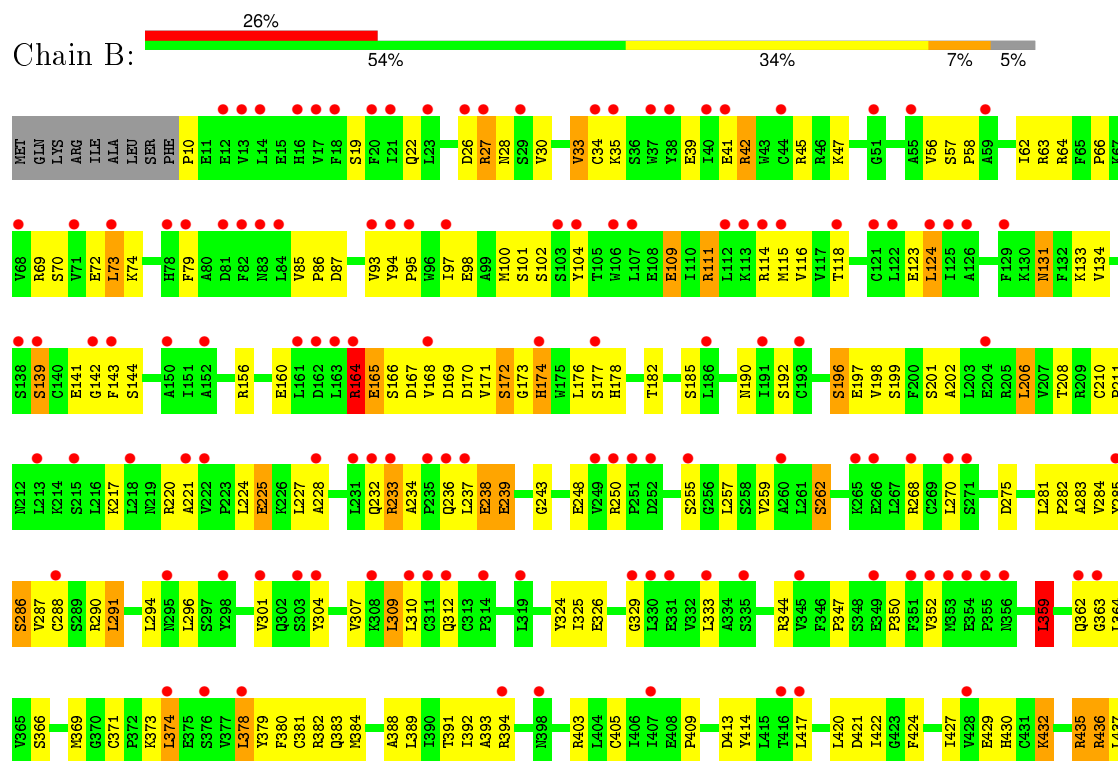
### 3 Residue-property plots

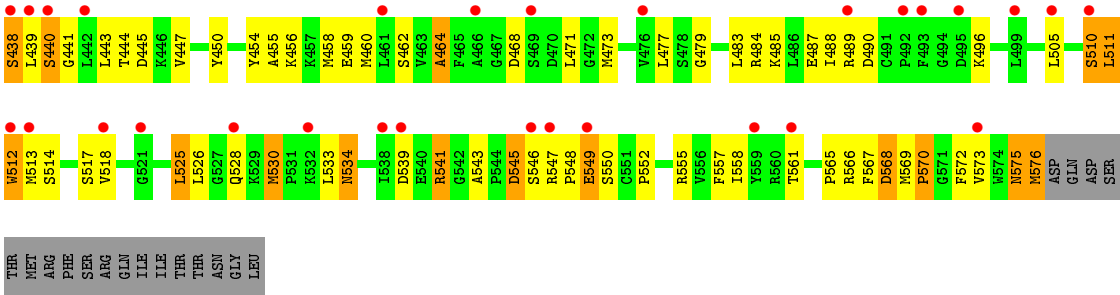
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.79Å 80.39Å 125.21Å 90.00° 104.72° 90.00°	Depositor
Resolution (Å)	49.71 – 2.70 49.71 – 2.70	Depositor EDS
% Data completeness (in resolution range)	47.8 (49.71-2.70) 95.5 (49.71-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.180 , 0.261 0.385 , 0.412	Depositor DCC
$R_{free}$ test set	1324 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	61.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 26077 reflections	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 2S3

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	0.75	0/728	0.77	0/982
2	B	1.30	16/4558 (0.4%)	1.20	30/6178 (0.5%)
All	All	1.24	16/5286 (0.3%)	1.15	30/7160 (0.4%)

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	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	512	TRP	CZ2-CH2	32.95	2.00	1.37
2	B	512	TRP	CD1-NE1	15.46	1.64	1.38
2	B	512	TRP	CG-CD2	13.82	1.67	1.43
2	B	512	TRP	CG-CD1	-10.62	1.21	1.36
2	B	512	TRP	CD2-CE2	8.32	1.51	1.41
2	B	512	TRP	CA-C	7.43	1.72	1.52
2	B	225	GLU	CG-CD	7.36	1.62	1.51
2	B	239	GLU	CB-CG	7.26	1.66	1.52
2	B	512	TRP	CD2-CE3	7.10	1.50	1.40
2	B	239	GLU	CD-OE2	7.08	1.33	1.25
2	B	512	TRP	CA-CB	6.86	1.69	1.53
2	B	511	LEU	C-O	6.68	1.36	1.23
2	B	512	TRP	CZ3-CH2	6.65	1.50	1.40
2	B	464	ALA	CA-CB	-6.07	1.39	1.52
2	B	512	TRP	C-O	5.60	1.33	1.23
2	B	239	GLU	CG-CD	5.49	1.60	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	512	TRP	CG-CD2-CE3	-20.39	115.55	133.90
2	B	512	TRP	NE1-CE2-CD2	-11.36	95.94	107.30
2	B	512	TRP	CE2-CD2-CG	10.30	115.54	107.30
2	B	512	TRP	CA-CB-CG	-9.63	95.40	113.70
2	B	512	TRP	CH2-CZ2-CE2	-9.40	108.00	117.40
2	B	512	TRP	CE2-CD2-CE3	8.50	128.90	118.70
2	B	512	TRP	CD1-NE1-CE2	8.30	116.47	109.00
2	B	512	TRP	CB-CA-C	8.18	126.76	110.40
2	B	512	TRP	CD1-CG-CD2	-7.90	99.98	106.30
2	B	512	TRP	N-CA-C	-7.89	89.69	111.00
2	B	526	LEU	CB-CG-CD2	-7.35	98.51	111.00
2	B	421	ASP	CB-CG-OD1	6.86	124.47	118.30
2	B	511	LEU	CA-C-O	-6.81	105.81	120.10
2	B	436	ARG	NE-CZ-NH2	6.67	123.63	120.30
2	B	512	TRP	NE1-CE2-CZ2	6.54	137.59	130.40
2	B	513	MET	N-CA-C	-6.40	93.71	111.00
2	B	359	LEU	CA-CB-CG	-6.16	101.14	115.30
2	B	525	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	420	LEU	CB-CG-CD1	-6.07	100.67	111.00
2	B	220	ARG	NE-CZ-NH1	-5.93	117.33	120.30
2	B	435	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	B	511	LEU	N-CA-CB	-5.50	99.40	110.40
2	B	250	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	B	73	LEU	CA-CB-CG	5.42	127.76	115.30
2	B	243	GLY	N-CA-C	-5.27	99.92	113.10
2	B	510	SER	CA-C-O	-5.10	109.39	120.10
2	B	533	LEU	CB-CG-CD1	-5.09	102.34	111.00
2	B	233	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	B	479	GLY	N-CA-C	5.05	125.71	113.10
2	B	568	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	LEU	Peptide
1	A	104	ALA	Peptide
1	A	28	THR	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	721	0	731	118	0
2	B	4461	0	4504	200	6
3	B	36	0	5	6	0
4	B	16	0	14	8	0
5	A	37	0	0	11	2
5	B	264	0	0	58	3
All	All	5535	0	5254	321	7

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 31.

All (321) 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:101:LEU:HD13	1:A:102:ILE:CD1	1.41	1.49
2:B:512:TRP:CZ2	2:B:512:TRP:CH2	1.99	1.48
1:A:29:ILE:CG2	1:A:30:ALA:H	1.18	1.46
1:A:101:LEU:HD22	1:A:102:ILE:N	1.48	1.28
1:A:29:ILE:CG2	1:A:30:ALA:N	1.86	1.22
2:B:576:MET:O	5:B:1006:HOH:O	1.56	1.19
1:A:102:ILE:HD13	1:A:102:ILE:N	1.54	1.17
2:B:569:MET:HE1	5:B:1088:HOH:O	1.40	1.16
1:A:102:ILE:H	1:A:102:ILE:CD1	1.56	1.15
4:B:1001:2S3:CAI	4:B:1001:2S3:HAH	1.79	1.12
1:A:106:ASN:O	1:A:108:LEU:N	1.83	1.12
4:B:1001:2S3:CAH	4:B:1001:2S3:HAIA	1.84	1.08
1:A:101:LEU:HD13	1:A:102:ILE:HD12	1.15	1.07
1:A:101:LEU:CD1	1:A:102:ILE:CD1	2.30	1.07
1:A:29:ILE:HG23	1:A:30:ALA:N	1.64	1.06
2:B:66:PRO:HB3	5:B:1047:HOH:O	1.57	1.03
1:A:29:ILE:HG22	1:A:30:ALA:N	1.52	1.03
2:B:10:PRO:HB2	5:B:1091:HOH:O	1.57	1.02
2:B:109:GLU:HB3	2:B:134:VAL:HB	1.43	1.01
1:A:26:SER:O	1:A:29:ILE:CG2	2.12	0.97
1:A:101:LEU:N	1:A:103:LEU:HG	1.82	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:VAL:HA	5:B:1256:HOH:O	1.66	0.95
1:A:101:LEU:N	1:A:103:LEU:HD21	1.80	0.95
1:A:101:LEU:N	1:A:103:LEU:CG	2.30	0.94
1:A:101:LEU:CD2	1:A:102:ILE:N	2.30	0.94
1:A:101:LEU:N	1:A:103:LEU:CD2	2.30	0.94
1:A:101:LEU:HD13	1:A:102:ILE:HD13	1.49	0.94
4:B:1001:2S3:HAH	4:B:1001:2S3:HAIA	0.94	0.93
1:A:26:SER:O	1:A:29:ILE:HG22	1.66	0.92
1:A:103:LEU:HD23	1:A:103:LEU:H	1.32	0.91
1:A:28:THR:HG21	1:A:107:TYR:O	1.71	0.91
2:B:432:LYS:HZ3	2:B:432:LYS:HB2	1.37	0.89
1:A:102:ILE:HD13	1:A:102:ILE:H	0.74	0.88
1:A:160:GLU:HG3	2:B:28:ASN:ND2	1.88	0.88
2:B:22:GLN:O	2:B:47:LYS:NZ	2.07	0.88
1:A:101:LEU:O	1:A:104:ALA:HB3	1.73	0.87
1:A:130:PRO:HD2	5:A:191:HOH:O	1.72	0.86
1:A:28:THR:OG1	1:A:108:LEU:HA	1.75	0.86
2:B:576:MET:O	5:B:1237:HOH:O	1.93	0.86
1:A:29:ILE:HG22	1:A:30:ALA:H	0.69	0.85
1:A:101:LEU:CD2	1:A:101:LEU:C	2.46	0.84
2:B:362:GLN:HB2	5:B:1218:HOH:O	1.79	0.83
1:A:101:LEU:HB3	1:A:102:ILE:HD13	1.59	0.83
2:B:73:LEU:HB3	2:B:115:MET:HE1	1.62	0.82
2:B:432:LYS:NZ	2:B:432:LYS:HB2	1.93	0.82
2:B:309:LEU:HD23	2:B:309:LEU:O	1.80	0.82
1:A:101:LEU:C	1:A:101:LEU:HD22	2.01	0.81
1:A:101:LEU:CB	1:A:102:ILE:HD13	2.10	0.81
1:A:101:LEU:HD22	1:A:102:ILE:H	1.41	0.80
4:B:1001:2S3:CAH	4:B:1001:2S3:CAI	2.52	0.80
2:B:111:ARG:HH11	2:B:111:ARG:HG2	1.47	0.79
1:A:101:LEU:O	1:A:104:ALA:CB	2.30	0.79
1:A:56:ILE:C	1:A:58:TYR:H	1.89	0.77
2:B:389:LEU:HG	5:B:1264:HOH:O	1.85	0.76
2:B:144:SER:HB3	2:B:169:ASP:HB3	1.65	0.76
4:B:1001:2S3:CAJ	4:B:1001:2S3:CAH	2.62	0.76
1:A:101:LEU:HB3	1:A:102:ILE:CD1	2.15	0.75
2:B:352:VAL:O	2:B:382:ARG:NH2	2.18	0.75
2:B:63:ARG:HB3	5:B:1071:HOH:O	1.84	0.75
1:A:101:LEU:HD13	1:A:102:ILE:HD11	1.63	0.75
2:B:255:SER:O	2:B:259:VAL:HG23	1.85	0.75
2:B:384:MET:SD	5:B:1264:HOH:O	2.46	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:281:LEU:O	2:B:284:VAL:HG22	1.88	0.74
1:A:101:LEU:CG	1:A:102:ILE:HD13	2.19	0.73
2:B:233:ARG:HD2	5:B:1111:HOH:O	1.86	0.73
2:B:288:CYS:HB3	2:B:312:GLN:HB2	1.70	0.73
2:B:394:ARG:HD2	5:B:1152:HOH:O	1.88	0.72
1:A:160:GLU:HG3	2:B:28:ASN:HD22	1.53	0.72
2:B:73:LEU:HB3	2:B:115:MET:CE	2.20	0.72
1:A:106:ASN:O	1:A:107:TYR:C	2.29	0.71
2:B:10:PRO:HD2	5:B:1089:HOH:O	1.88	0.71
2:B:284:VAL:O	2:B:287:VAL:HB	1.90	0.71
1:A:28:THR:O	1:A:29:ILE:HD13	1.91	0.70
2:B:459:GLU:OE1	2:B:484:ARG:NH1	2.24	0.70
2:B:545:ASP:HB3	5:B:1192:HOH:O	1.90	0.70
1:A:101:LEU:CD1	1:A:102:ILE:HD13	2.12	0.70
1:A:104:ALA:O	1:A:106:ASN:C	2.30	0.69
1:A:27:GLN:O	1:A:27:GLN:HG3	1.93	0.69
2:B:566:ARG:NH1	2:B:568:ASP:OD1	2.26	0.68
2:B:111:ARG:HH11	2:B:111:ARG:CG	2.07	0.68
1:A:104:ALA:C	1:A:106:ASN:N	2.47	0.68
2:B:409:PRO:HA	5:B:1029:HOH:O	1.92	0.68
2:B:72:GLU:HB2	5:B:1151:HOH:O	1.92	0.67
1:A:10:SER:HA	5:A:167:HOH:O	1.94	0.67
2:B:178:HIS:NE2	5:B:1014:HOH:O	1.67	0.67
1:A:102:ILE:HG23	1:A:117:THR:OG1	1.95	0.67
2:B:174:HIS:O	2:B:178:HIS:HD2	1.76	0.67
2:B:325:ILE:HG13	2:B:329:GLY:HA3	1.76	0.67
2:B:389:LEU:N	5:B:1264:HOH:O	2.25	0.67
2:B:39:GLU:OE2	2:B:42:ARG:NH1	2.28	0.67
1:A:102:ILE:C	1:A:104:ALA:H	1.97	0.66
2:B:94:TYR:HB3	2:B:95:PRO:HD3	1.78	0.66
2:B:185:SER:O	5:B:1031:HOH:O	2.13	0.66
2:B:287:VAL:CG1	2:B:291:LEU:HD13	2.26	0.65
1:A:101:LEU:O	1:A:103:LEU:N	2.30	0.65
1:A:108:LEU:O	1:A:109:ASN:HB2	1.95	0.65
1:A:56:ILE:O	1:A:58:TYR:N	2.30	0.65
1:A:101:LEU:O	1:A:104:ALA:N	2.30	0.65
2:B:539:ASP:OD2	2:B:541:ARG:HD2	1.97	0.65
2:B:286:SER:HB3	5:B:1223:HOH:O	1.98	0.65
2:B:534:ASN:HD21	2:B:565:PRO:HA	1.62	0.64
1:A:104:ALA:O	1:A:106:ASN:N	2.30	0.64
1:A:102:ILE:O	1:A:104:ALA:N	2.30	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:LEU:HD11	2:B:380:PHE:CE1	2.31	0.64
2:B:232:GLN:HG3	5:B:1079:HOH:O	1.96	0.64
2:B:285:TYR:HA	2:B:288:CYS:SG	2.37	0.64
2:B:422:ILE:HG12	5:B:1080:HOH:O	1.97	0.63
1:A:144:THR:OG1	1:A:147:GLU:HG3	1.98	0.63
2:B:393:ALA:HB2	2:B:427:ILE:HD13	1.81	0.63
2:B:505:LEU:HD13	2:B:558:ILE:HG21	1.81	0.63
4:B:1001:2S3:CAH	4:B:1001:2S3:HAJA	2.29	0.63
2:B:281:LEU:HD11	2:B:301:VAL:HG21	1.80	0.62
1:A:28:THR:O	1:A:29:ILE:CD1	2.47	0.62
1:A:129:THR:HB	5:A:191:HOH:O	1.99	0.62
2:B:484:ARG:HG2	5:B:1099:HOH:O	1.99	0.62
1:A:48:THR:HG22	1:A:51:ILE:HD13	1.80	0.62
1:A:101:LEU:O	1:A:102:ILE:C	2.36	0.61
1:A:106:ASN:C	1:A:108:LEU:N	2.54	0.61
2:B:70:SER:OG	2:B:109:GLU:HG3	2.00	0.61
2:B:27:ARG:HB3	2:B:45:ARG:NH2	2.15	0.61
2:B:403:ARG:HG2	2:B:438:SER:HB3	1.81	0.61
1:A:101:LEU:C	1:A:103:LEU:N	2.50	0.60
2:B:512:TRP:NE1	2:B:514:SER:HB3	2.15	0.60
1:A:135:THR:HG22	1:A:136:THR:N	2.17	0.60
2:B:447:VAL:O	2:B:450:TYR:HB2	2.02	0.60
2:B:359:LEU:HD21	2:B:379:TYR:CZ	2.37	0.60
2:B:176:LEU:HD21	2:B:206:LEU:HD12	1.83	0.59
1:A:102:ILE:HG23	1:A:117:THR:CB	2.33	0.58
2:B:414:TYR:HB2	5:B:1201:HOH:O	2.02	0.58
1:A:120:THR:O	1:A:123:ASP:HB2	2.04	0.58
2:B:281:LEU:HB2	2:B:282:PRO:HD3	1.84	0.58
1:A:26:SER:O	1:A:29:ILE:HG21	2.01	0.58
1:A:102:ILE:C	1:A:104:ALA:N	2.57	0.58
1:A:27:GLN:HB3	1:A:109:ASN:HD22	1.69	0.58
2:B:64:ARG:NH2	5:B:1133:HOH:O	2.27	0.57
2:B:378:LEU:HD11	2:B:380:PHE:HE1	1.66	0.57
2:B:512:TRP:HE1	2:B:514:SER:CB	2.17	0.57
1:A:107:TYR:CD2	1:A:108:LEU:HD23	2.40	0.57
2:B:42:ARG:HB2	2:B:64:ARG:O	2.05	0.57
2:B:66:PRO:HA	5:B:1047:HOH:O	2.05	0.57
2:B:63:ARG:HG3	5:B:1085:HOH:O	2.05	0.57
1:A:56:ILE:C	1:A:58:TYR:N	2.57	0.56
1:A:48:THR:HG22	1:A:51:ILE:CD1	2.35	0.56
2:B:485:LYS:NZ	3:B:1000:IHP:O31	2.37	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:THR:HB	5:A:175:HOH:O	2.04	0.56
2:B:160:GLU:CG	5:B:1105:HOH:O	2.53	0.56
2:B:324:TYR:O	2:B:326:GLU:HG3	2.04	0.56
2:B:171:VAL:O	2:B:172:SER:HB3	2.06	0.56
2:B:131:ASN:O	2:B:133:LYS:HG3	2.06	0.56
2:B:539:ASP:O	2:B:572:PHE:HB2	2.06	0.55
2:B:100:MET:HG2	2:B:104:TYR:CD1	2.41	0.55
2:B:445:ASP:OD1	2:B:468:ASP:HB2	2.07	0.55
2:B:66:PRO:CA	5:B:1047:HOH:O	2.54	0.54
2:B:10:PRO:HD3	5:B:1247:HOH:O	2.07	0.54
2:B:94:TYR:CE1	2:B:124:LEU:HD12	2.42	0.54
1:A:106:ASN:C	1:A:108:LEU:H	2.10	0.54
2:B:378:LEU:HD12	2:B:378:LEU:C	2.27	0.54
1:A:29:ILE:O	1:A:30:ALA:O	2.26	0.54
2:B:262:SER:HB3	2:B:286:SER:HB3	1.87	0.54
2:B:512:TRP:HE1	2:B:514:SER:HB3	1.70	0.54
1:A:160:GLU:C	5:A:169:HOH:O	2.46	0.54
2:B:94:TYR:CE2	2:B:98:GLU:HG3	2.43	0.54
2:B:174:HIS:O	2:B:178:HIS:CD2	2.60	0.54
2:B:234:ALA:HB1	2:B:237:LEU:HD13	1.90	0.54
2:B:93:VAL:HG12	2:B:116:VAL:O	2.07	0.54
1:A:101:LEU:CD2	1:A:102:ILE:H	2.11	0.53
2:B:454:TYR:O	2:B:456:LYS:N	2.42	0.53
2:B:144:SER:CB	2:B:169:ASP:HB3	2.38	0.53
2:B:86:PRO:HG3	5:B:1251:HOH:O	2.07	0.53
1:A:153:ARG:HD2	5:A:194:HOH:O	2.08	0.53
2:B:239:GLU:HB3	5:B:1018:HOH:O	2.09	0.53
2:B:287:VAL:HG12	2:B:291:LEU:HD13	1.91	0.52
2:B:19:SER:O	2:B:22:GLN:NE2	2.42	0.52
2:B:62:ILE:HD13	5:B:1027:HOH:O	2.09	0.52
1:A:103:LEU:H	1:A:103:LEU:CD2	2.04	0.51
2:B:288:CYS:CB	2:B:312:GLN:HB2	2.39	0.51
2:B:288:CYS:HA	2:B:291:LEU:HD22	1.92	0.51
2:B:236:GLN:OE1	2:B:236:GLN:N	2.37	0.51
1:A:101:LEU:C	1:A:101:LEU:HD23	2.28	0.51
2:B:282:PRO:HA	2:B:285:TYR:CZ	2.46	0.51
2:B:484:ARG:NH2	3:B:1000:IHP:O31	2.42	0.51
2:B:441:GLY:O	2:B:443:LEU:HG	2.10	0.51
2:B:97:ILE:O	2:B:101:SER:HB3	2.10	0.51
1:A:106:ASN:O	1:A:109:ASN:N	2.44	0.51
3:B:1000:IHP:O44	3:B:1000:IHP:O33	2.29	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:GLU:HG3	5:B:1105:HOH:O	2.09	0.51
2:B:405:CYS:HB2	4:B:1001:2S3:HAI	1.93	0.51
2:B:190:ASN:HA	2:B:217:LYS:HB2	1.93	0.50
2:B:63:ARG:NE	5:B:1109:HOH:O	2.44	0.50
1:A:102:ILE:CG2	1:A:117:THR:OG1	2.60	0.50
1:A:126:LYS:HB3	5:A:164:HOH:O	2.11	0.50
2:B:347:PRO:HG2	2:B:350:PRO:HG3	1.93	0.50
1:A:48:THR:CG2	1:A:51:ILE:CD1	2.90	0.50
2:B:62:ILE:HG22	5:B:1216:HOH:O	2.12	0.49
2:B:66:PRO:CB	5:B:1047:HOH:O	2.32	0.49
2:B:388:ALA:HB3	5:B:1264:HOH:O	2.12	0.49
1:A:27:GLN:O	1:A:27:GLN:CG	2.60	0.49
2:B:569:MET:O	2:B:570:PRO:O	2.30	0.49
2:B:287:VAL:CG1	2:B:291:LEU:CD1	2.90	0.49
2:B:224:LEU:HD11	2:B:257:LEU:HD11	1.95	0.49
2:B:309:LEU:HD23	2:B:309:LEU:C	2.29	0.49
3:B:1000:IHP:O23	5:B:1044:HOH:O	2.19	0.49
1:A:20:GLU:O	1:A:20:GLU:HG2	2.12	0.49
2:B:569:MET:CE	2:B:575:ASN:HB2	2.42	0.49
2:B:413:ASP:OD1	2:B:413:ASP:C	2.50	0.49
2:B:569:MET:SD	2:B:573:VAL:HG12	2.53	0.49
2:B:464:ALA:HB2	4:B:1001:2S3:HAD	1.95	0.49
2:B:164:ARG:O	2:B:166:SER:N	2.46	0.49
2:B:530:MET:HE2	5:B:1052:HOH:O	2.13	0.49
1:A:104:ALA:O	1:A:105:ALA:C	2.51	0.48
1:A:160:GLU:HG3	2:B:28:ASN:HD21	1.75	0.48
2:B:359:LEU:HD21	2:B:379:TYR:OH	2.13	0.48
2:B:304:TYR:O	2:B:307:VAL:HB	2.13	0.48
2:B:570:PRO:HG2	2:B:573:VAL:CG2	2.44	0.48
2:B:517:SER:C	5:B:1115:HOH:O	2.51	0.48
2:B:118:THR:HA	2:B:142:GLY:O	2.14	0.48
2:B:290:ARG:NH2	5:B:1256:HOH:O	2.46	0.48
2:B:569:MET:C	2:B:570:PRO:O	2.50	0.48
2:B:114:ARG:HA	2:B:139:SER:O	2.14	0.47
2:B:487:GLU:C	2:B:488:ILE:HG13	2.34	0.47
2:B:436:ARG:HD2	2:B:460:MET:HE3	1.96	0.47
2:B:383:GLN:HG2	5:B:1053:HOH:O	2.14	0.47
1:A:101:LEU:CD1	1:A:102:ILE:HD11	2.32	0.47
1:A:103:LEU:HD23	1:A:103:LEU:N	2.15	0.47
2:B:325:ILE:O	2:B:329:GLY:HA3	2.13	0.47
2:B:512:TRP:CZ2	2:B:555:ARG:HD3	2.49	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:569:MET:CE	5:B:1088:HOH:O	2.22	0.47
2:B:312:GLN:NE2	5:B:1095:HOH:O	2.48	0.47
2:B:460:MET:CE	5:B:1016:HOH:O	2.62	0.47
1:A:137:PHE:HB3	1:A:138:ASN:H	1.49	0.47
1:A:101:LEU:HD22	1:A:102:ILE:HD13	1.97	0.47
1:A:107:TYR:CD2	1:A:108:LEU:CD2	2.98	0.47
2:B:257:LEU:HA	2:B:257:LEU:HD23	1.81	0.47
2:B:294:LEU:HD21	2:B:296:LEU:HD11	1.97	0.46
2:B:79:PHE:CE2	2:B:489:ARG:HD3	2.50	0.46
2:B:510:SER:HB2	2:B:557:PHE:CE1	2.51	0.46
1:A:121:VAL:C	1:A:123:ASP:N	2.69	0.46
2:B:310:LEU:HD13	2:B:333:LEU:HD13	1.97	0.46
2:B:429:GLU:HB2	5:B:1259:HOH:O	2.15	0.46
2:B:518:VAL:O	2:B:552:PRO:HA	2.16	0.46
1:A:101:LEU:CD1	1:A:102:ILE:HD12	2.10	0.46
2:B:19:SER:HB3	5:B:1030:HOH:O	2.15	0.46
2:B:74:LYS:NZ	3:B:1000:IHP:H1	2.31	0.46
2:B:143:PHE:CE1	2:B:168:VAL:HG22	2.50	0.46
1:A:160:GLU:CG	2:B:28:ASN:HD22	2.27	0.46
2:B:170:ASP:OD1	2:B:196:SER:HB3	2.15	0.46
2:B:57:SER:O	2:B:58:PRO:C	2.55	0.45
2:B:543:ALA:O	2:B:546:SER:OG	2.28	0.45
2:B:570:PRO:HG2	2:B:573:VAL:HG23	1.97	0.45
2:B:545:ASP:C	2:B:547:ARG:H	2.18	0.45
2:B:202:ALA:O	2:B:206:LEU:HB2	2.17	0.45
2:B:569:MET:HE3	2:B:575:ASN:HB2	1.98	0.45
1:A:101:LEU:HD22	1:A:102:ILE:CA	2.40	0.45
2:B:238:GLU:C	2:B:239:GLU:HG3	2.36	0.45
1:A:137:PHE:O	1:A:138:ASN:HB2	2.16	0.45
2:B:437:LEU:HG	2:B:438:SER:N	2.32	0.45
2:B:33:VAL:O	2:B:34:CYS:HB3	2.16	0.45
1:A:138:ASN:ND2	1:A:138:ASN:O	2.50	0.45
1:A:119:GLN:O	1:A:123:ASP:OD2	2.34	0.45
2:B:262:SER:HB3	2:B:286:SER:CB	2.46	0.45
1:A:125:ILE:O	1:A:126:LYS:C	2.53	0.45
2:B:548:PRO:O	2:B:550:SER:N	2.49	0.45
1:A:107:TYR:HD2	1:A:108:LEU:CD2	2.30	0.44
1:A:101:LEU:CD2	1:A:102:ILE:HD13	2.47	0.44
2:B:228:ALA:HB3	5:B:1005:HOH:O	2.17	0.44
1:A:44:LEU:HD13	1:A:47:VAL:HG21	1.99	0.44
1:A:149:GLU:CB	5:A:189:HOH:O	2.64	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:SER:HA	5:A:173:HOH:O	2.18	0.44
1:A:121:VAL:C	1:A:123:ASP:H	2.20	0.44
1:A:149:GLU:HB3	5:A:162:HOH:O	2.17	0.44
1:A:102:ILE:HA	1:A:105:ALA:HB3	2.00	0.43
2:B:109:GLU:CB	2:B:134:VAL:HB	2.31	0.43
2:B:63:ARG:HD2	5:B:1209:HOH:O	2.17	0.43
1:A:155:ASN:OD1	2:B:64:ARG:NH2	2.36	0.43
2:B:210:CYS:HA	2:B:211:PRO:HD2	1.85	0.43
2:B:197:GLU:HG3	2:B:221:ALA:HB1	2.00	0.43
2:B:363:GLY:O	2:B:366:SER:HB2	2.19	0.43
2:B:10:PRO:C	5:B:1091:HOH:O	2.56	0.43
2:B:94:TYR:HE2	2:B:98:GLU:OE1	2.01	0.43
2:B:382:ARG:HG3	2:B:382:ARG:HH11	1.83	0.43
1:A:28:THR:HG23	1:A:108:LEU:O	2.18	0.43
2:B:525:LEU:O	2:B:528:GLN:HB2	2.19	0.43
2:B:208:THR:HG23	5:B:1235:HOH:O	2.19	0.43
2:B:545:ASP:C	2:B:547:ARG:N	2.72	0.43
2:B:239:GLU:CB	5:B:1018:HOH:O	2.67	0.43
2:B:424:PHE:CD2	2:B:439:LEU:HD23	2.54	0.42
1:A:149:GLU:HB2	5:A:189:HOH:O	2.19	0.42
1:A:48:THR:CG2	1:A:51:ILE:HD12	2.48	0.42
2:B:489:ARG:HD2	5:B:1048:HOH:O	2.19	0.42
2:B:382:ARG:HG3	2:B:382:ARG:NH1	2.34	0.42
2:B:30:VAL:HG23	2:B:41:GLU:HG3	2.02	0.42
2:B:104:TYR:HA	5:B:1090:HOH:O	2.19	0.42
2:B:435:ARG:HA	2:B:458:MET:HA	2.02	0.42
2:B:285:TYR:N	5:B:1239:HOH:O	2.52	0.42
2:B:344:ARG:HG2	2:B:378:LEU:HB3	2.01	0.42
1:A:143:PHE:HB3	1:A:148:GLU:HB2	2.02	0.42
2:B:444:THR:HB	2:B:468:ASP:OD2	2.20	0.42
1:A:20:GLU:OE1	1:A:24:LEU:HD11	2.18	0.42
2:B:56:VAL:HG22	2:B:57:SER:N	2.35	0.42
2:B:374:LEU:HA	2:B:374:LEU:HD23	1.93	0.42
2:B:62:ILE:HG21	5:B:1027:HOH:O	2.20	0.41
1:A:101:LEU:N	1:A:103:LEU:CD1	2.82	0.41
2:B:270:LEU:HD12	2:B:291:LEU:HD21	2.01	0.41
2:B:405:CYS:HA	2:B:440:SER:OG	2.20	0.41
2:B:288:CYS:HB3	2:B:312:GLN:CB	2.45	0.41
2:B:287:VAL:HG13	2:B:291:LEU:HD13	1.97	0.41
3:B:1000:IHP:O25	3:B:1000:IHP:O16	2.38	0.41
2:B:173:GLY:HA3	2:B:197:GLU:O	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LYS:HB3	1:A:10:SER:H	1.65	0.41
2:B:496:LYS:HG3	2:B:496:LYS:HZ3	1.76	0.41
2:B:371:CYS:O	2:B:373:LYS:N	2.53	0.41
2:B:473:MET:HE2	2:B:511:LEU:HD21	2.03	0.41
1:A:22:VAL:HG13	1:A:22:VAL:O	2.21	0.41
1:A:127:GLY:HA2	2:B:26:ASP:OD1	2.21	0.41
1:A:101:LEU:HB3	1:A:102:ILE:HD11	1.99	0.41
2:B:85:VAL:HG22	2:B:512:TRP:CH2	2.56	0.41
2:B:178:HIS:NE2	5:B:1231:HOH:O	2.37	0.41
2:B:391:THR:O	2:B:392:ILE:C	2.60	0.41
2:B:477:LEU:HA	2:B:477:LEU:HD23	1.77	0.41
1:A:44:LEU:HA	1:A:45:PRO:HD3	1.97	0.40
2:B:268:ARG:HA	2:B:268:ARG:HD3	1.81	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:PRO:CD	2:B:567:PHE:CE1[2_656]	1.62	0.58
5:A:166:HOH:O	5:B:1065:HOH:O[3_545]	1.78	0.42
2:B:567:PHE:O	5:B:1083:HOH:O[2_656]	1.81	0.39
2:B:565:PRO:CG	2:B:567:PHE:CD1[2_656]	1.83	0.37
2:B:417:LEU:CD1	5:B:1119:HOH:O[3_455]	1.92	0.28
2:B:430:HIS:CE1	5:A:166:HOH:O[3_455]	2.01	0.19
2:B:565:PRO:CG	2:B:567:PHE:CE1[2_656]	2.06	0.14

## 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	82/160 (51%)	58 (71%)	10 (12%)	14 (17%)	<b>0</b> <b>0</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	565/594 (95%)	508 (90%)	47 (8%)	10 (2%)	11	27
All	All	647/754 (86%)	566 (88%)	57 (9%)	24 (4%)	4	9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ALA
1	A	29	ILE
1	A	57	GLU
1	A	105	ALA
1	A	107	TYR
2	B	165	GLU
2	B	570	PRO
1	A	102	ILE
1	A	103	LEU
1	A	109	ASN
1	A	138	ASN
2	B	549	GLU
1	A	106	ASN
1	A	135	THR
1	A	136	THR
2	B	225	GLU
2	B	455	ALA
2	B	164	ARG
2	B	172	SER
2	B	283	ALA
1	A	145	PRO
2	B	196	SER
1	A	45	PRO
2	B	131	ASN

### 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	81/137 (59%)	67 (83%)	14 (17%)	2	6
2	B	500/525 (95%)	446 (89%)	54 (11%)	8	18
All	All	581/662 (88%)	513 (88%)	68 (12%)	7	15

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ILE
1	A	47	VAL
1	A	51	ILE
1	A	101	LEU
1	A	102	ILE
1	A	103	LEU
1	A	111	LYS
1	A	114	LEU
1	A	120	THR
1	A	124	MET
1	A	137	PHE
1	A	139	ILE
1	A	145	PRO
1	A	153	ARG
2	B	27	ARG
2	B	33	VAL
2	B	35	LYS
2	B	42	ARG
2	B	69	ARG
2	B	87	ASP
2	B	102	SER
2	B	109	GLU
2	B	111	ARG
2	B	123	GLU
2	B	124	LEU
2	B	139	SER
2	B	141	GLU
2	B	156	ARG
2	B	164	ARG
2	B	165	GLU
2	B	167	ASP
2	B	174	HIS
2	B	177	SER
2	B	182	THR
2	B	192	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	198	VAL
2	B	199	SER
2	B	201	SER
2	B	206	LEU
2	B	227	LEU
2	B	238	GLU
2	B	248	GLU
2	B	262	SER
2	B	275	ASP
2	B	286	SER
2	B	291	LEU
2	B	309	LEU
2	B	359	LEU
2	B	364	LEU
2	B	369	MET
2	B	374	LEU
2	B	378	LEU
2	B	381	CYS
2	B	432	LYS
2	B	438	SER
2	B	440	SER
2	B	462	SER
2	B	471	LEU
2	B	483	LEU
2	B	490	ASP
2	B	530	MET
2	B	534	ASN
2	B	541	ARG
2	B	545	ASP
2	B	549	GLU
2	B	561	THR
2	B	575	ASN
2	B	576	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
2	B	178	HIS
2	B	312	GLN
2	B	317	GLN

### 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 carbohydrates 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$
3	IHP	B	1000	-	36,36,36	0.90	1 (2%)	48,60,60	3.24	27 (56%)
4	2S3	B	1001	-	13,17,17	1.65	3 (23%)	14,23,23	1.76	5 (35%)

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
3	IHP	B	1000	-	-	0/30/54/54	0/1/1/1
4	2S3	B	1001	-	-	0/4/11/11	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	2S3	CAN-CAP	-2.01	1.38	1.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	2S3	CAD-CAF	2.59	1.42	1.36
3	B	1000	IHP	P3-O13	2.63	1.68	1.60
4	B	1001	2S3	CAH-CAN	4.07	1.45	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1000	IHP	C4-C3-C2	-5.67	97.89	110.43
3	B	1000	IHP	P6-O16-C6	-5.66	107.99	121.56
3	B	1000	IHP	P4-O14-C4	-3.70	112.69	121.56
3	B	1000	IHP	C6-C1-C2	-3.66	102.34	110.43
4	B	1001	2S3	CAH-CAN-CAQ	-2.85	119.51	126.74
4	B	1001	2S3	CAM-CAQ-CAN	-2.59	107.43	111.26
4	B	1001	2S3	CAE-CAG-CAP	-2.17	117.81	120.88
4	B	1001	2S3	CAF-CAO-CAP	-2.14	117.45	121.11
3	B	1000	IHP	O12-P2-O22	-2.13	101.79	107.11
3	B	1000	IHP	O14-C4-C5	2.02	113.15	108.47
3	B	1000	IHP	O44-P4-O34	2.02	115.08	107.38
3	B	1000	IHP	O42-P2-O22	2.10	117.34	110.58
3	B	1000	IHP	O34-P4-O24	2.11	117.39	110.58
3	B	1000	IHP	P3-O13-C3	2.25	126.95	121.56
3	B	1000	IHP	O45-P5-O35	2.35	116.34	107.38
3	B	1000	IHP	O46-P6-O36	2.51	116.92	107.38
4	B	1001	2S3	CAE-CAD-CAF	2.87	124.62	120.45
3	B	1000	IHP	C5-C6-C1	2.94	116.93	110.43
3	B	1000	IHP	O43-P3-O23	3.14	120.69	110.58
3	B	1000	IHP	O16-C6-C1	3.26	116.03	108.47
3	B	1000	IHP	O11-P1-O21	3.32	115.40	107.11
3	B	1000	IHP	C5-C4-C3	3.66	118.52	110.43
3	B	1000	IHP	O14-C4-C3	3.69	117.02	108.47
3	B	1000	IHP	O16-C6-C5	4.06	117.88	108.47
3	B	1000	IHP	O15-C5-C6	4.24	118.31	108.47
3	B	1000	IHP	O11-C1-C2	4.27	118.39	108.47
3	B	1000	IHP	O11-C1-C6	4.64	119.23	108.47
3	B	1000	IHP	C6-C5-C4	4.76	120.95	110.43
3	B	1000	IHP	P5-O15-C5	5.17	133.97	121.56
3	B	1000	IHP	O12-C2-C3	6.38	123.28	108.47
3	B	1000	IHP	C3-C2-C1	6.65	125.14	110.43
3	B	1000	IHP	O13-C3-C2	8.66	128.56	108.47

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	IHP	6	0
4	B	1001	2S3	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	90/160 (56%)	2.62	47 (52%) <b>0</b> <b>0</b>	29, 59, 69, 70	0
2	B	567/594 (95%)	1.52	156 (27%) <b>1</b> <b>1</b>	25, 41, 56, 73	0
All	All	657/754 (87%)	1.67	203 (30%) <b>1</b> <b>0</b>	25, 42, 63, 73	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	131	GLU	9.3
1	A	135	THR	9.2
1	A	9	LYS	9.2
2	B	17	VAL	8.4
2	B	232	GLN	8.0
1	A	43	PRO	7.9
1	A	139	ILE	7.7
2	B	94	TYR	7.7
2	B	311	CYS	7.5
1	A	50	LYS	7.0
1	A	48	THR	6.9
1	A	44	LEU	6.8
1	A	47	VAL	6.8
1	A	116	LEU	6.6
2	B	288	CYS	6.5
1	A	136	THR	6.3
1	A	28	THR	6.0
1	A	138	ASN	5.9
2	B	168	VAL	5.9
1	A	56	ILE	5.9
1	A	134	ARG	5.8
2	B	352	VAL	5.8
2	B	107	LEU	5.8
2	B	83	ASN	5.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	416	THR	5.7
2	B	398	ASN	5.6
2	B	260	ALA	5.6
2	B	12	GLU	5.5
2	B	37	TRP	5.4
2	B	521	GLY	5.2
2	B	78	HIS	5.2
2	B	125	ILE	5.0
2	B	547	ARG	4.9
2	B	97	ILE	4.8
1	A	140	LYS	4.7
2	B	221	ALA	4.7
2	B	14	LEU	4.6
2	B	126	ALA	4.5
2	B	539	ASP	4.5
2	B	362	GLN	4.5
2	B	439	LEU	4.5
2	B	13	VAL	4.4
2	B	222	VAL	4.3
2	B	73	LEU	4.3
1	A	118	CYS	4.3
2	B	252	ASP	4.3
2	B	476	VAL	4.3
2	B	356	ASN	4.3
2	B	231	LEU	4.3
2	B	21	ILE	4.2
2	B	93	VAL	4.2
2	B	40	ILE	4.2
2	B	213	LEU	4.1
2	B	251	PRO	4.1
2	B	301	VAL	4.1
2	B	308	LYS	4.0
1	A	51	ILE	4.0
2	B	469	SER	4.0
1	A	137	PHE	4.0
2	B	18	PHE	3.9
1	A	30	ALA	3.8
2	B	495	ASP	3.8
2	B	351	PHE	3.8
2	B	41	GLU	3.7
1	A	52	LEU	3.7
2	B	353	MET	3.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	204	GLU	3.7
1	A	57	GLU	3.7
2	B	466	ALA	3.6
1	A	8	LEU	3.6
2	B	35	LYS	3.6
2	B	118	THR	3.5
1	A	58	TYR	3.5
1	A	122	ALA	3.5
2	B	193	CYS	3.4
2	B	354	GLU	3.4
2	B	499	LEU	3.4
2	B	573	VAL	3.4
2	B	298	TYR	3.4
2	B	271	SER	3.4
2	B	68	VAL	3.4
1	A	114	LEU	3.3
2	B	363	GLY	3.3
2	B	71	VAL	3.3
2	B	270	LEU	3.2
2	B	549	GLU	3.2
2	B	122	LEU	3.2
2	B	124	LEU	3.2
2	B	268	ARG	3.2
2	B	112	LEU	3.2
2	B	295	ASN	3.2
1	A	24	LEU	3.2
2	B	355	PRO	3.1
1	A	141	ASN	3.1
2	B	27	ARG	3.1
2	B	561	THR	3.0
2	B	177	SER	3.0
2	B	218	LEU	3.0
2	B	329	GLY	3.0
1	A	117	THR	3.0
2	B	546	SER	3.0
2	B	191	ILE	3.0
2	B	121	CYS	2.9
1	A	53	ALA	2.9
2	B	331	GLU	2.9
1	A	26	SER	2.9
2	B	26	ASP	2.9
2	B	20	PHE	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	142	GLY	2.9
2	B	303	SER	2.9
2	B	59	ALA	2.9
2	B	312	GLN	2.9
2	B	407	ILE	2.8
2	B	333	LEU	2.8
2	B	55	ALA	2.8
2	B	518	VAL	2.8
2	B	152	ALA	2.8
2	B	79	PHE	2.8
2	B	51	GLY	2.8
2	B	440	SER	2.8
1	A	45	PRO	2.8
2	B	29	SER	2.8
2	B	215	SER	2.7
1	A	130	PRO	2.7
2	B	378	LEU	2.7
2	B	103	SER	2.7
2	B	34	CYS	2.7
2	B	310	LEU	2.7
2	B	266	GLU	2.7
2	B	538	ILE	2.7
2	B	114	ARG	2.7
1	A	49	SER	2.7
2	B	115	MET	2.7
1	A	143	PHE	2.7
1	A	55	VAL	2.6
1	A	150	GLU	2.6
2	B	44	CYS	2.6
1	A	133	ILE	2.6
2	B	236	GLN	2.6
2	B	138	SER	2.6
2	B	374	LEU	2.5
2	B	489	ARG	2.5
2	B	330	LEU	2.5
2	B	255	SER	2.5
2	B	510	SER	2.5
2	B	164	ARG	2.5
2	B	249	VAL	2.5
2	B	235	PRO	2.5
2	B	174	HIS	2.5
1	A	142	ASP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	161	LEU	2.4
2	B	528	GLN	2.4
2	B	143	PHE	2.4
2	B	335	SER	2.4
2	B	250	ARG	2.4
2	B	38	TYR	2.3
2	B	304	TYR	2.3
2	B	162	ASP	2.3
1	A	120	THR	2.3
2	B	376	SER	2.3
1	A	29	ILE	2.3
2	B	428	VAL	2.3
2	B	265	LYS	2.3
2	B	559	TYR	2.3
2	B	113	LYS	2.3
2	B	163	LEU	2.3
2	B	319	LEU	2.3
2	B	492	PRO	2.2
2	B	16	HIS	2.2
2	B	150	ALA	2.2
2	B	345	VAL	2.2
2	B	81	ASP	2.2
2	B	186	LEU	2.2
2	B	505	LEU	2.2
2	B	82	PHE	2.2
2	B	438	SER	2.2
1	A	27	GLN	2.2
2	B	349	GLU	2.2
2	B	104	TYR	2.2
2	B	394	ARG	2.2
1	A	103	LEU	2.1
2	B	129	PHE	2.1
2	B	228	ALA	2.1
2	B	237	LEU	2.1
2	B	417	LEU	2.1
1	A	10	SER	2.1
1	A	125	ILE	2.1
2	B	139	SER	2.1
1	A	112	ASN	2.1
2	B	84	LEU	2.1
2	B	461	LEU	2.1
2	B	532	LYS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	512	TRP	2.1
2	B	442	LEU	2.1
2	B	95	PRO	2.1
2	B	106	TRP	2.1
2	B	233	ARG	2.1
2	B	285	TYR	2.1
2	B	493	PHE	2.0
1	A	23	ALA	2.0
2	B	23	LEU	2.0
2	B	513	MET	2.0
2	B	314	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	2S3	B	1001	16/16	0.53	0.56	2.47	77,80,84,85	0
3	IHP	B	1000	36/36	0.75	0.27	-0.57	67,78,99,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.