

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	7XGX
Title	:	Glucosyltransferase
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Deposited on	:	2022-04-07
Resolution	:	2.39 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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) 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	:	2.35
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)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.39 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	А	655	4% 58%	29%	5%• 7%			
1	В	655	5%	32%	5% • 10%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9711 atoms, of which 44 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	607	Total	С	Ν	Ο	S	0	0	0
1		001	4801	3040	828	907	26	0		
1	D	501	Total	С	Ν	0	\mathbf{S}	0	0	0
	I D	591	4674	2964	802	882	26	0	U	

• Molecule 1 is a protein called Lgt2.

There are 38 of	discrepancies	between	the modelled	and reference	sequences:
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Chain	Residue	Modelled	Actual	Comment	Reference
А	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
А	-17	GLY	-	expression tag	UNP A0A2S6F0H5
А	-16	SER	-	expression tag	UNP A0A2S6F0H5
А	-15	SER	-	expression tag	UNP A0A2S6F0H5
А	-14	HIS	-	expression tag	UNP A0A2S6F0H5
А	-13	HIS	-	expression tag	UNP A0A2S6F0H5
А	-12	HIS	-	expression tag	UNP A0A2S6F0H5
А	-11	HIS	-	expression tag	UNP A0A2S6F0H5
А	-10	HIS	-	expression tag	UNP A0A2S6F0H5
А	-9	HIS	-	expression tag	UNP A0A2S6F0H5
А	-8	SER	-	expression tag	UNP A0A2S6F0H5
А	-7	SER	-	expression tag	UNP A0A2S6F0H5
А	-6	GLY	-	expression tag	UNP A0A2S6F0H5
А	-5	LEU	-	expression tag	UNP A0A2S6F0H5
А	-4	VAL	-	expression tag	UNP A0A2S6F0H5
А	-3	PRO	-	expression tag	UNP A0A2S6F0H5
А	-2	ARG	-	expression tag	UNP A0A2S6F0H5
А	-1	GLY	-	expression tag	UNP A0A2S6F0H5
А	0	SER	-	expression tag	UNP A0A2S6F0H5
В	-18	MET	-	initiating methionine	UNP A0A2S6F0H5
В	-17	GLY	-	expression tag	UNP A0A2S6F0H5
В	-16	SER	-	expression tag	UNP A0A2S6F0H5
В	-15	SER	-	expression tag	UNP A0A2S6F0H5
В	-14	HIS	-	expression tag	UNP A0A2S6F0H5
В	-13	HIS	-	expression tag	UNP A0A2S6F0H5



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Chain	Residue	Modelled	Actual	Comment	Reference
В	-12	HIS	-	expression tag	UNP A0A2S6F0H5
В	-11	HIS	-	expression tag	UNP A0A2S6F0H5
В	-10	HIS	-	expression tag	UNP A0A2S6F0H5
В	-9	HIS	-	expression tag	UNP A0A2S6F0H5
В	-8	SER	-	expression tag	UNP A0A2S6F0H5
В	-7	SER	-	expression tag	UNP A0A2S6F0H5
В	-6	GLY	-	expression tag	UNP A0A2S6F0H5
В	-5	LEU	-	expression tag	UNP A0A2S6F0H5
В	-4	VAL	-	expression tag	UNP A0A2S6F0H5
В	-3	PRO	-	expression tag	UNP A0A2S6F0H5
В	-2	ARG	-	expression tag	UNP A0A2S6F0H5
В	-1	GLY	-	expression tag	UNP A0A2S6F0H5
В	0	SER	-	expression tag	UNP A0A2S6F0H5

• Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf			
0		1	Total	С	Η	Ν	Ο	Р	0	0	
Z A	1	58	15	22	2	17	2	0	0		
0	D	В	1	Total	С	Η	Ν	Ο	Р	0	0
2 B	1	58	15	22	2	17	2	0	U		

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	52	$\begin{array}{cc} \text{Total} & \text{O} \\ 52 & 52 \end{array}$	0	0
3	В	68	Total O 68 68	0	0



3 Residue-property plots (i)

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: Lgt2





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.06Å 75.86Å 126.64Å	Deneriten
a, b, c, α , β , γ	90.00° 90.24° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	32.22 - 2.39	Depositor
Resolution (A)	$75.05 \ - \ 2.39$	EDS
% Data completeness	95.3 (32.22-2.39)	Depositor
(in resolution range)	94.1 (75.05-2.39)	EDS
R _{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.50 (at 2.40 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
P. P.	0.215 , 0.265	Depositor
Π, Π_{free}	0.226 , 0.257	DCC
R_{free} test set	1988 reflections (3.57%)	wwPDB-VP
Wilson B-factor $(Å^2)$	49.9	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34 , 46.6	EDS
L-test for twinning ²	$< L > = 0.47, < L^2 > = 0.30$	Xtriage
	0.013 for -k,-h,-l	
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
	0.149 for h,-k,-l	
F_o, F_c correlation	0.95	EDS
Total number of atoms	9711	wwPDB-VP
Average B, all atoms $(Å^2)$	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.62% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: UPG

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).

Mal	Chain	Bond lengths		Bond angles	
Moi Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.82	1/4887~(0.0%)	0.74	9/6603~(0.1%)
1	В	0.77	0/4760	0.81	17/6435~(0.3%)
All	All	0.79	1/9647~(0.0%)	0.77	26/13038~(0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	303	GLU	CD-OE2	-5.10	1.20	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	47	ASP	N-CA-C	15.61	153.15	111.00
1	А	29	LYS	CB-CA-C	-15.39	79.61	110.40
1	В	47	ASP	CB-CA-C	-14.67	81.06	110.40
1	В	17	ASN	CB-CA-C	12.65	135.70	110.40
1	А	5	TYR	CB-CA-C	-11.64	87.12	110.40
1	В	133	GLU	N-CA-C	-9.56	85.18	111.00
1	А	632	ALA	CB-CA-C	8.60	122.99	110.10
1	В	133	GLU	CB-CA-C	8.44	127.28	110.40
1	А	109	PHE	N-CA-C	8.40	133.68	111.00
1	В	73	ILE	N-CA-C	8.06	132.77	111.00
1	В	565	THR	CB-CA-C	-7.85	90.40	111.60
1	В	46	ASN	CB-CA-C	7.82	126.04	110.40
1	В	133	GLU	C-N-CD	-7.72	103.63	120.60
1	А	5	TYR	N-CA-C	7.25	130.57	111.00
1	В	17	ASN	N-CA-C	-7.04	91.98	111.00
1	A	46	ASN	CB-CA-C	6.91	124.22	110.40
1	В	284	PHE	CB-CA-C	-6.77	96.86	110.40
1	A	41	ASN	N-CA-C	6.32	128.05	111.00



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	565	THR	N-CA-C	6.30	128.01	111.00
1	В	565	THR	N-CA-C	6.11	127.49	111.00
1	В	132	ASP	N-CA-C	6.07	127.39	111.00
1	А	632	ALA	C-N-CA	5.84	136.31	121.70
1	В	521	LEU	CB-CG-CD1	5.68	120.66	111.00
1	В	73	ILE	CB-CA-C	-5.40	100.81	111.60
1	В	158	GLN	CB-CA-C	5.15	120.69	110.40
1	В	248	ASN	N-CA-C	5.10	124.78	111.00

There are no chirality outliers.

There are no planarity outliers.

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	А	4801	0	4854	234	0
1	В	4674	0	4717	276	0
2	А	36	22	22	1	0
2	В	36	22	22	1	0
3	А	52	0	0	2	0
3	В	68	0	0	5	0
All	All	9667	44	9615	510	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 27.

All (510) 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:129:ILE:CD1	1:A:192:THR:HG23	1.49	1.41
1:B:249:ALA:CB	1:B:250:PRO:CD	2.15	1.23
1:B:249:ALA:CB	1:B:250:PRO:HD2	1.71	1.21
1:B:249:ALA:HB1	1:B:250:PRO:CD	1.70	1.19
1:A:129:ILE:CD1	1:A:192:THR:CG2	2.20	1.19
1:A:114:VAL:HG12	1:A:172:ILE:HG22	1.25	1.15



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:129:ILE:HD12	1:A:192:THR:CG2	1.81	1.11
1:B:249:ALA:HB1	1:B:250:PRO:HD3	1.27	1.11
1:B:109:PHE:CD1	1:B:167:ARG:HA	1.86	1.09
1:B:249:ALA:HB3	1:B:250:PRO:HD2	1.30	1.07
1:A:17:ASN:OD1	1:A:20:GLU:HG2	1.52	1.07
1:A:129:ILE:HD11	1:A:192:THR:CG2	1.84	1.02
1:A:105:ALA:HB1	1:A:166:ILE:HD11	1.43	1.00
1:A:515:MET:HA	1:A:518:VAL:HG13	1.39	1.00
1:A:543:LYS:HB3	1:A:544:PRO:HD3	1.42	1.00
1:B:567:GLU:HG2	1:B:568:PRO:HD2	1.43	1.00
1:B:44:PHE:HD1	1:B:44:PHE:N	1.55	0.98
1:B:482:VAL:HG23	1:B:510:TYR:CB	1.92	0.97
1:A:129:ILE:HD11	1:A:192:THR:HG23	1.00	0.96
1:A:247:GLN:CD	1:A:345:THR:HG21	1.87	0.95
1:B:126:CYS:HB3	1:B:134:PRO:HG3	1.48	0.94
1:B:140:GLU:HG2	1:B:374:VAL:HG23	1.49	0.94
1:B:482:VAL:HG23	1:B:510:TYR:HB3	1.47	0.93
1:B:24:LEU:HD23	1:B:61:PHE:HE2	1.34	0.90
1:B:515:MET:HA	1:B:518:VAL:HG12	1.54	0.90
1:B:562:LEU:HG	1:B:582:ILE:HD11	1.52	0.89
1:A:104:GLY:O	1:A:108:THR:HG23	1.71	0.89
1:A:19:ASN:O	1:A:23:ARG:HB2	1.72	0.88
1:B:626:TRP:HB2	3:B:807:HOH:O	1.72	0.88
1:B:18:GLN:O	1:B:22:THR:HG23	1.76	0.85
1:A:567:GLU:HG2	1:A:568:PRO:HD2	1.59	0.84
1:B:567:GLU:HG2	1:B:568:PRO:CD	2.08	0.84
1:B:478:PHE:O	1:B:482:VAL:HG12	1.77	0.83
1:A:249:ALA:HB1	1:A:250:PRO:HD3	1.59	0.83
1:B:46:ASN:O	1:B:373:GLY:HA2	1.79	0.83
1:B:167:ARG:HG3	1:B:168:ASP:N	1.92	0.83
1:A:23:ARG:NE	1:A:61:PHE:CE1	2.45	0.83
1:A:486:GLU:OE1	1:A:486:GLU:N	2.11	0.82
1:B:284:PHE:CG	1:B:284:PHE:O	2.34	0.81
1:A:109:PHE:O	1:A:109:PHE:CD1	2.33	0.81
1:A:18:GLN:O	1:A:22:THR:HG23	1.80	0.81
1:B:8:PHE:O	1:B:12:THR:HB	1.82	0.79
1:B:452:LEU:HB3	1:B:453:PRO:HD3	1.64	0.79
1:A:518:VAL:HA	1:A:521:LEU:HD23	1.65	0.79
1:B:24:LEU:HD23	1:B:61:PHE:CE2	2.19	0.78
1:B:29:LYS:O	1:B:30:ARG:HD3	1.84	0.78
1:A:567:GLU:HG2	1:A:568:PRO:CD	2.13	0.78



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:513:HIS:CD2	1:A:513:HIS:H	2.01	0.78	
1:A:114:VAL:HG12	1:A:172:ILE:CG2	2.11	0.77	
1:A:24:LEU:CD1	1:A:28:LEU:HD22	2.15	0.77	
1:B:109:PHE:CE1	1:B:167:ARG:HB2	2.20	0.77	
1:B:129:ILE:HD11	1:B:188:LYS:O	1.86	0.76	
1:B:73:ILE:HG22	1:B:73:ILE:O	1.84	0.76	
1:B:109:PHE:CE1	1:B:167:ARG:CB	2.68	0.76	
1:B:109:PHE:HE1	1:B:167:ARG:CB	1.99	0.76	
1:B:154:TYR:HE2	1:B:179:ILE:HG21	1.50	0.76	
1:A:444:GLU:OE2	1:A:444:GLU:HA	1.86	0.76	
1:B:162:LEU:O	1:B:166:ILE:HG22	1.86	0.75	
1:B:543:LYS:HB3	1:B:544:PRO:HD3	1.66	0.75	
1:B:429:ARG:HD3	1:B:477:ARG:HH12	1.51	0.75	
1:A:426:GLU:OE1	1:A:429:ARG:NH1	2.20	0.74	
1:B:109:PHE:CE1	1:B:167:ARG:HA	2.22	0.74	
1:A:249:ALA:HB1	1:A:250:PRO:CD	2.18	0.74	
1:B:429:ARG:HG2	1:B:477:ARG:NH2	2.03	0.74	
1:A:114:VAL:CG1	1:A:172:ILE:HG22	2.12	0.74	
1:B:135:ASN:ND2	1:B:138:GLN:H	1.86	0.74	
1:A:247:GLN:OE1	1:A:345:THR:CG2	2.36	0.73	
1:B:429:ARG:HG2	1:B:477:ARG:HH22	1.53	0.73	
1:A:172:ILE:HG13	1:A:172:ILE:O	1.89	0.73	
1:B:542:TYR:CD2	1:B:628:PRO:HG3	2.23	0.73	
1:A:515:MET:HA	1:A:518:VAL:CG1	2.17	0.73	
1:A:67:TRP:HE1	1:A:71:GLN:HE21	1.35	0.72	
1:A:442:ASP:O	1:A:446:ASN:HB2	1.89	0.72	
1:B:29:LYS:HE2	1:B:42:LYS:HE2	1.69	0.72	
1:A:24:LEU:HD13	1:A:28:LEU:HD22	1.70	0.71	
1:A:24:LEU:HD23	1:A:61:PHE:HE2	1.54	0.71	
1:A:249:ALA:CB	1:A:250:PRO:CD	2.68	0.71	
1:B:477:ARG:HE	1:B:481:MET:CE	2.03	0.71	
1:A:175:LYS:HB3	1:A:178:GLU:HG2	1.72	0.71	
1:A:508:VAL:HG21	1:A:526:LYS:HG2	1.73	0.71	
1:A:627:MET:HE3	1:A:628:PRO:HD3	1.72	0.71	
1:B:46:ASN:O	1:B:373:GLY:CA	2.38	0.71	
1:A:109:PHE:CD1	1:A:109:PHE:C	2.64	0.71	
1:A:6:TRP:CZ2	1:A:40:ILE:HB	2.26	0.71	
1:A:567:GLU:OE1	1:A:568:PRO:O	2.08	0.71	
1:A:23:ARG:O	1:A:26:THR:HG22	1.92	0.70	
1:B:126:CYS:CB	1:B:134:PRO:HG3	2.21	0.70	
1:B:154:TYR:CD1	1:B:158:GLN:HG2	2.27	0.69	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:513:HIS:H	1:B:513:HIS:CD2	2.08	0.69
1:B:543:LYS:HB3	1:B:544:PRO:CD	2.22	0.69
1:B:155:SER:H	1:B:158:GLN:HE22	1.40	0.68
1:B:196:ASN:C	1:B:196:ASN:HD22	1.96	0.68
1:B:117:LEU:HD21	1:B:177:GLU:HG2	1.75	0.68
1:A:155:SER:O	1:A:158:GLN:NE2	2.22	0.68
1:A:627:MET:HE3	1:A:628:PRO:CD	2.24	0.68
1:A:521:LEU:HD12	1:A:525:GLU:HG3	1.77	0.67
1:B:515:MET:HA	1:B:518:VAL:CG1	2.24	0.67
1:A:109:PHE:C	1:A:109:PHE:HD1	1.97	0.67
1:B:41:ASN:CG	1:B:41:ASN:O	2.32	0.67
1:B:112:SER:OG	1:B:166:ILE:HD12	1.95	0.67
1:A:110:GLY:HA2	1:A:115:VAL:HG11	1.76	0.66
1:B:522:ASN:OD1	1:B:522:ASN:N	2.26	0.66
1:A:42:LYS:O	1:A:42:LYS:HD3	1.95	0.66
1:A:624:LEU:HD22	2:A:701:UPG:O1B	1.94	0.66
1:A:73:ILE:O	1:A:76:ASN:HB2	1.96	0.66
1:A:247:GLN:CD	1:A:345:THR:CG2	2.64	0.66
1:B:109:PHE:CE1	1:B:167:ARG:CA	2.78	0.66
1:B:379:GLU:HG2	1:B:583:LEU:CD1	2.26	0.66
1:A:247:GLN:OE1	1:A:345:THR:HG23	1.95	0.66
1:A:109:PHE:CE1	1:A:111:LYS:HB2	2.31	0.66
1:B:44:PHE:N	1:B:44:PHE:CD1	2.29	0.66
1:A:23:ARG:O	1:A:26:THR:CG2	2.44	0.65
1:A:609:SER:O	1:A:613:VAL:HG23	1.96	0.65
1:A:116:LYS:HD2	1:A:116:LYS:C	2.17	0.65
1:B:117:LEU:HD23	1:B:176:PHE:HE1	1.62	0.65
1:A:238:LYS:O	1:A:242:GLU:HG3	1.96	0.65
1:B:186:ARG:HH21	1:B:189:GLU:HB3	1.62	0.65
1:B:162:LEU:O	1:B:162:LEU:HD12	1.96	0.65
1:B:562:LEU:HG	1:B:582:ILE:CD1	2.25	0.65
1:A:614:GLU:HA	1:A:614:GLU:OE1	1.96	0.65
1:B:109:PHE:HD1	1:B:167:ARG:HA	1.56	0.64
1:B:158:GLN:OE1	1:B:159:ALA:N	2.31	0.64
1:B:129:ILE:HG12	1:B:191:HIS:HB2	1.78	0.64
1:B:135:ASN:OD1	1:B:138:GLN:NE2	2.29	0.64
1:A:46:ASN:O	1:A:47:ASP:OD2	2.13	0.64
1:A:129:ILE:CD1	1:A:192:THR:HG21	2.24	0.64
1:A:17:ASN:O	1:A:21:ALA:CB	2.46	0.64
1:B:482:VAL:HG23	1:B:510:TYR:HB2	1.80	0.64
1:B:154:TYR:CE2	1:B:179:ILE:HG21	2.31	0.64



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:104:GLY:HA2	1:A:107:ILE:CG2	2.28	0.63	
1:B:129:ILE:HG13	1:B:192:THR:HG23	1.81	0.63	
1:B:201:ASN:O	1:B:562:LEU:HD13	1.97	0.63	
1:B:370:VAL:CG1	1:B:378:MET:HB2	2.28	0.63	
1:A:292:GLU:OE2	1:A:402:LYS:HE3	1.99	0.63	
1:A:259:ARG:NH2	1:A:264:LYS:HG3	2.13	0.63	
1:B:42:LYS:HA	1:B:44:PHE:CE1	2.34	0.63	
1:A:319:SER:OG	1:A:323:ARG:NH2	2.30	0.62	
1:A:482:VAL:CG2	1:A:507:LEU:HA	2.29	0.62	
1:B:444:GLU:HB3	3:B:829:HOH:O	1.99	0.62	
1:A:129:ILE:HD12	1:A:192:THR:HG21	1.79	0.61	
1:A:475:VAL:HG21	1:A:492:GLN:HE21	1.65	0.61	
1:B:117:LEU:HD23	1:B:176:PHE:CE1	2.34	0.61	
1:A:170:LYS:HB2	1:A:171:PRO:HD2	1.81	0.61	
1:B:543:LYS:CB	1:B:544:PRO:CD	2.78	0.61	
1:A:24:LEU:O	1:A:28:LEU:N	2.31	0.61	
1:A:154:TYR:CE2	1:A:162:LEU:HD13	2.35	0.61	
1:B:53:LEU:O	1:B:57:MET:HB2	2.01	0.61	
1:B:123:ARG:NH2	1:B:133:GLU:OE1	2.34	0.61	
1:B:430:LEU:HD23	1:B:541:LEU:HD13	1.82	0.61	
1:A:105:ALA:CB	1:A:166:ILE:HD11	2.27	0.60	
1:B:479:ALA:HB1	1:B:485:PRO:HA	1.84	0.60	
1:A:23:ARG:HE	1:A:61:PHE:HE1	1.36	0.60	
1:B:359:HIS:CG	1:B:360:PRO:HD2	2.37	0.60	
1:A:257:TYR:CE1	1:A:281:LEU:HG	2.36	0.60	
1:B:605:ASN:O	1:B:608:THR:HG22	2.01	0.60	
1:A:66:GLU:OE2	1:A:66:GLU:HA	2.01	0.60	
1:B:484:ALA:HB1	1:B:486:GLU:OE1	2.02	0.59	
1:A:117:LEU:O	1:A:117:LEU:HG	2.02	0.59	
1:B:272:GLN:O	1:B:276:GLU:HG3	2.02	0.59	
1:A:452:LEU:HB3	1:A:453:PRO:HD3	1.83	0.59	
1:A:606:TRP:O	1:A:607:ILE:HG12	2.01	0.59	
1:B:43:LEU:H	1:B:43:LEU:HD22	1.67	0.59	
1:B:222:CYS:SG	1:B:241:LEU:HD21	2.42	0.59	
1:A:155:SER:C	1:A:158:GLN:HE22	2.05	0.59	
1:B:515:MET:O	1:B:518:VAL:HG13	2.03	0.59	
1:B:369:LEU:O	1:B:610:SER:HB2	2.02	0.59	
1:A:359:HIS:CG	1:A:360:PRO:HD2	2.37	0.59	
1:A:367:SER:OG	1:A:607:ILE:N	2.31	0.59	
1:B:74:LEU:O	1:B:77:ILE:HD12	2.02	0.59	
1:B:367:SER:OG	1:B:607:ILE:N	2.31	0.58	



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:529:LEU:HA	1:B:532:LYS:NZ	2.18	0.58
1:B:529:LEU:HA	1:B:532:LYS:HZ3	1.69	0.58
1:B:528:ASN:O	1:B:532:LYS:HD3	2.02	0.58
1:A:515:MET:HG2	1:A:518:VAL:CG2	2.33	0.58
1:A:324:TRP:CE2	1:A:404:ILE:HG21	2.39	0.58
1:A:40:ILE:CG2	1:A:44:PHE:HE1	2.17	0.58
1:A:318:ALA:O	1:A:322:VAL:HG23	2.04	0.57
1:B:482:VAL:HG21	1:B:506:ALA:O	2.03	0.57
1:B:513:HIS:CD2	1:B:513:HIS:N	2.72	0.57
1:A:625:SER:O	1:A:631:GLN:NE2	2.36	0.57
1:A:494:ALA:HB1	1:A:499:ASN:HB3	1.87	0.57
1:A:17:ASN:O	1:A:21:ALA:HB2	2.04	0.57
1:A:417:GLU:O	1:A:421:LYS:HG3	2.04	0.57
1:A:161:LYS:HZ3	1:A:173:PRO:HG2	1.70	0.57
1:A:164:GLU:HG3	1:A:167:ARG:HH11	1.68	0.57
1:B:238:LYS:O	1:B:242:GLU:HG3	2.04	0.57
1:A:162:LEU:O	1:A:166:ILE:HG23	2.04	0.57
1:A:513:HIS:H	1:A:513:HIS:HD2	1.51	0.57
1:B:516:ASP:O	1:B:519:SER:HB3	2.05	0.56
1:B:129:ILE:HG13	1:B:192:THR:CG2	2.34	0.56
1:A:148:LEU:O	1:A:148:LEU:HD23	2.06	0.56
1:B:186:ARG:NH2	1:B:189:GLU:HB3	2.20	0.56
1:B:546:VAL:HA	3:B:842:HOH:O	2.05	0.56
1:A:24:LEU:HD12	1:A:28:LEU:HD22	1.88	0.56
1:A:513:HIS:CD2	1:A:513:HIS:N	2.72	0.56
1:A:40:ILE:HG21	1:A:44:PHE:HE1	1.71	0.56
1:A:148:LEU:O	1:A:152:GLU:HG2	2.06	0.56
1:B:129:ILE:HG12	1:B:191:HIS:CB	2.36	0.56
1:A:117:LEU:HD23	1:A:176:PHE:HE1	1.69	0.56
1:A:170:LYS:HB2	1:A:171:PRO:CD	2.35	0.56
1:B:140:GLU:HG2	1:B:374:VAL:CG2	2.32	0.56
1:B:174:SER:O	1:B:175:LYS:HG2	2.06	0.56
1:B:515:MET:CE	1:B:518:VAL:CG1	2.83	0.56
1:B:515:MET:CE	1:B:518:VAL:HG13	2.36	0.56
1:B:229:PRO:O	1:B:263:THR:HG23	2.06	0.56
1:B:605:ASN:O	1:B:608:THR:CG2	2.54	0.56
1:A:3:GLU:O	1:A:3:GLU:HG3	2.04	0.56
1:A:493:GLU:O	1:A:497:GLN:HG2	2.06	0.56
1:B:170:LYS:HB3	1:B:171:PRO:HD2	1.87	0.56
1:B:515:MET:HE2	1:B:518:VAL:HG11	1.88	0.56
1:B:222:CYS:SG	1:B:255:LEU:HD13	2.45	0.55



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:24:LEU:O	1:B:28:LEU:HB2	2.07	0.55
1:B:15:GLY:O	1:B:57:MET:HE2	2.06	0.55
1:B:186:ARG:HA	1:B:186:ARG:NE	2.21	0.55
1:A:161:LYS:HZ3	1:A:173:PRO:CG	2.19	0.55
1:A:499:ASN:O	1:A:502:VAL:HG13	2.07	0.55
1:B:78:GLN:HB2	1:B:79:PRO:HD2	1.87	0.54
1:B:446:ASN:O	1:B:447:ASN:O	2.25	0.54
1:A:477:ARG:O	1:A:481:MET:HG3	2.07	0.54
1:A:120:GLN:HE21	1:A:120:GLN:HA	1.72	0.54
1:A:142:ILE:O	1:A:146:LEU:HD22	2.06	0.54
1:B:513:HIS:H	1:B:513:HIS:HD2	1.52	0.54
1:A:161:LYS:NZ	1:A:173:PRO:HG2	2.23	0.54
1:A:17:ASN:OD1	1:A:20:GLU:CG	2.41	0.54
1:B:112:SER:OG	1:B:114:VAL:HG23	2.08	0.54
1:B:604:PRO:HB2	1:B:608:THR:HG21	1.90	0.54
1:B:515:MET:HG2	1:B:518:VAL:HG11	1.89	0.54
1:B:612:GLU:OE1	1:B:612:GLU:HA	2.08	0.53
1:A:556:THR:O	1:A:560:LEU:HG	2.08	0.53
1:B:284:PHE:O	1:B:284:PHE:CD1	2.61	0.53
1:A:259:ARG:HH22	1:A:264:LYS:HG3	1.71	0.53
1:B:56:TYR:O	1:B:58:ALA:N	2.41	0.53
1:B:109:PHE:CD1	1:B:167:ARG:CA	2.75	0.53
1:A:619:LEU:O	1:A:619:LEU:HD12	2.08	0.53
1:A:120:GLN:HA	1:A:120:GLN:NE2	2.24	0.53
1:A:494:ALA:CB	1:A:499:ASN:HB3	2.39	0.53
1:B:416:THR:CG2	1:B:450:LEU:HD23	2.39	0.53
1:B:446:ASN:O	1:B:447:ASN:C	2.46	0.53
1:B:493:GLU:O	1:B:497:GLN:HB2	2.09	0.53
1:B:515:MET:HE1	1:B:518:VAL:HG22	1.90	0.53
1:A:109:PHE:O	1:A:109:PHE:HD1	1.87	0.53
1:A:405:ALA:O	1:A:409:ILE:HG13	2.09	0.53
1:B:157:GLU:O	1:B:160:GLU:N	2.42	0.53
1:B:430:LEU:HD23	1:B:541:LEU:CD1	2.39	0.53
1:A:117:LEU:O	1:A:121:ASN:OD1	2.26	0.52
1:A:181:LEU:HB3	1:A:182:PRO:HD3	1.91	0.52
1:A:488:ALA:N	1:A:489:PRO:HD2	2.24	0.52
1:B:104:GLY:O	1:B:108:THR:HG23	2.09	0.52
1:B:434:PRO:HD2	1:B:474:GLY:N	2.24	0.52
1:B:514:GLY:O	1:B:517:ASN:HB2	2.09	0.52
1:A:195:LEU:HD12	1:A:579:ASP:O	2.09	0.52
1:B:109:PHE:HE1	1:B:167:ARG:HB2	1.62	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:117:LEU:O	1:B:121:ASN:HB2	2.09	0.52
1:A:117:LEU:HD23	1:A:176:PHE:CE1	2.45	0.52
1:B:227:ASN:HA	1:B:307:MET:HE3	1.91	0.52
1:B:265:LYS:HE2	3:B:849:HOH:O	2.09	0.52
1:B:363:LEU:CD1	1:B:559:ILE:HD11	2.40	0.52
1:A:470:VAL:O	1:A:473:ILE:O	2.28	0.52
1:B:236:LYS:H	1:B:236:LYS:CE	2.22	0.52
1:B:509:ALA:HB2	1:B:515:MET:HG2	1.92	0.52
1:A:611:GLU:CD	1:A:611:GLU:H	2.12	0.52
1:A:543:LYS:CB	1:A:544:PRO:HD3	2.22	0.51
1:A:125:ILE:HD11	1:A:184:VAL:HG13	1.92	0.51
1:A:543:LYS:HB3	1:A:544:PRO:CD	2.29	0.51
1:B:482:VAL:CG2	1:B:510:TYR:CB	2.80	0.51
1:A:6:TRP:CH2	1:A:40:ILE:HB	2.45	0.51
1:B:520:ARG:HD2	1:B:520:ARG:C	2.31	0.51
1:A:74:LEU:C	1:A:76:ASN:H	2.14	0.51
1:A:515:MET:HG2	1:A:518:VAL:HG22	1.93	0.51
1:B:186:ARG:HA	1:B:186:ARG:HE	1.76	0.51
1:B:370:VAL:HG13	1:B:378:MET:HB2	1.93	0.51
1:B:154:TYR:CE1	1:B:162:LEU:HD23	2.46	0.50
1:A:218:LYS:HD2	1:A:353:GLU:HG2	1.93	0.50
1:B:344:LEU:N	1:B:597:ASN:O	2.41	0.50
1:B:367:SER:O	1:B:608:THR:HG23	2.11	0.50
1:B:389:ASN:HB2	1:B:592:VAL:HG12	1.93	0.50
1:B:416:THR:HG22	1:B:450:LEU:HD23	1.94	0.50
1:B:433:MET:HE3	1:B:472:PHE:HD1	1.76	0.50
1:A:28:LEU:HD21	1:A:49:PHE:CZ	2.47	0.50
1:A:567:GLU:HG2	1:A:568:PRO:N	2.26	0.50
1:B:606:TRP:C	1:B:607:ILE:HG12	2.32	0.50
1:A:161:LYS:HZ1	1:A:162:LEU:HD12	1.76	0.50
1:A:516:ASP:OD1	1:A:517:ASN:N	2.45	0.50
1:B:314:ASN:ND2	3:B:807:HOH:O	2.44	0.49
1:B:135:ASN:O	1:B:136:LEU:C	2.49	0.49
1:B:434:PRO:HG2	1:B:474:GLY:HA2	1.93	0.49
1:B:73:ILE:O	1:B:75:SER:N	2.45	0.49
1:B:603:ILE:HB	1:B:604:PRO:HD2	1.95	0.49
1:B:52:ARG:NH1	1:B:80:LEU:HD21	2.28	0.49
1:B:567:GLU:CG	1:B:568:PRO:HD2	2.29	0.49
1:B:488:ALA:HB3	1:B:489:PRO:HD3	1.94	0.49
1:B:148:LEU:HD23	1:B:148:LEU:O	2.13	0.48
1:A:24:LEU:HD23	1:A:61:PHE:CE2	2.41	0.48



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:522:ASN:H	1:A:525:GLU:CD	2.17	0.48	
1:A:154:TYR:HB3	1:A:159:ALA:HB2	1.94	0.48	
1:A:348:LYS:HD2	1:A:348:LYS:HA	1.49	0.48	
1:A:520:ARG:HD2	1:A:520:ARG:N	2.29	0.48	
1:B:430:LEU:HD22	1:B:433:MET:HE2	1.95	0.48	
1:A:289:CYS:HB3	1:A:293:ASP:HB3	1.96	0.48	
1:A:504:THR:HG23	1:A:530:ILE:HD11	1.94	0.48	
1:B:140:GLU:HG3	1:B:144:ARG:HD2	1.96	0.48	
1:A:72:GLN:O	1:A:73:ILE:HG23	2.14	0.48	
1:B:125:ILE:HG12	1:B:188:LYS:HB2	1.95	0.48	
1:B:515:MET:HE2	1:B:518:VAL:CG1	2.44	0.48	
1:B:516:ASP:OD1	1:B:516:ASP:N	2.42	0.48	
1:B:606:TRP:O	1:B:607:ILE:HG12	2.14	0.48	
1:A:149:GLN:HA	1:A:149:GLN:OE1	2.13	0.48	
1:A:254:LYS:NZ	3:A:807:HOH:O	2.47	0.48	
1:A:296:LEU:HD11	1:A:405:ALA:CB	2.44	0.48	
1:A:109:PHE:O	1:A:109:PHE:CG	2.61	0.48	
1:A:395:LYS:O	1:A:399:ILE:HG13	2.14	0.48	
1:B:320:ASP:HB3	1:B:550:SER:O	2.14	0.48	
1:B:324:TRP:CE2	1:B:404:ILE:HG21	2.49	0.48	
1:A:170:LYS:CB	1:A:171:PRO:CD	2.91	0.47	
1:A:429:ARG:HD3	1:A:477:ARG:NH2	2.28	0.47	
1:B:74:LEU:CD2	1:B:77:ILE:HD11	2.45	0.47	
1:B:141:TYR:CD1	1:B:570:ARG:HD2	2.49	0.47	
1:B:155:SER:H	1:B:158:GLN:NE2	2.09	0.47	
1:A:433:MET:SD	1:A:473:ILE:HG22	2.54	0.47	
1:B:433:MET:HE3	1:B:472:PHE:CD1	2.48	0.47	
1:A:5:TYR:O	1:A:5:TYR:CG	2.65	0.47	
1:A:515:MET:CA	1:A:518:VAL:HG13	2.28	0.47	
1:A:20:GLU:HA	1:A:23:ARG:HB2	1.97	0.47	
1:A:194:ILE:HD11	1:A:577:GLN:NE2	2.29	0.47	
1:A:42:LYS:HD3	1:A:42:LYS:C	2.34	0.47	
1:B:470:VAL:O	1:B:473:ILE:O	2.33	0.47	
1:B:516:ASP:O	1:B:519:SER:CB	2.62	0.47	
1:B:604:PRO:HB2	1:B:608:THR:CG2	2.44	0.47	
1:B:259:ARG:HH22	1:B:264:LYS:HG3	1.80	0.47	
1:A:416:THR:HG22	1:A:450:LEU:HD23	1.97	0.47	
1:B:40:ILE:O	1:B:42:LYS:N	2.44	0.47	
1:B:374:VAL:HG23	1:B:374:VAL:O	2.15	0.47	
1:B:126:CYS:O	1:B:130:LEU:HG	2.15	0.47	
1:A:114:VAL:CG2	1:A:166:ILE:HG22	2.45	0.46	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:626:TRP:HA	1:A:631:GLN:CG	2.45	0.46	
1:A:627:MET:HE3	1:A:628:PRO:HD2	1.96	0.46	
1:B:130:LEU:O	1:B:576:LYS:HG3	2.15	0.46	
1:B:501:ILE:HD12	1:B:501:ILE:H	1.81	0.46	
1:A:126:CYS:HB3	1:A:134:PRO:CG	2.45	0.46	
1:B:356:TYR:O	1:B:595:LYS:NZ	2.40	0.46	
1:B:465:ASN:ND2	1:B:468:SER:OG	2.40	0.46	
1:B:482:VAL:CG2	1:B:510:TYR:HB2	2.45	0.46	
1:A:235:LYS:HE2	1:A:239:ASP:OD1	2.16	0.46	
1:A:259:ARG:HB2	1:A:283:ASP:OD2	2.15	0.46	
1:B:234:PRO:HB3	1:B:236:LYS:NZ	2.30	0.46	
1:A:164:GLU:HG3	1:A:167:ARG:NH1	2.31	0.46	
1:B:122:ALA:HB2	1:B:146:LEU:HD12	1.97	0.46	
1:B:154:TYR:HD1	1:B:158:GLN:HG2	1.79	0.46	
1:A:482:VAL:O	1:A:482:VAL:HG13	2.16	0.46	
1:B:227:ASN:HA	1:B:307:MET:CE	2.46	0.46	
1:A:104:GLY:CA	1:A:107:ILE:HG22	2.46	0.46	
1:B:236:LYS:H	1:B:236:LYS:HE2	1.80	0.46	
1:B:433:MET:CE	1:B:472:PHE:CD1	2.99	0.46	
1:B:129:ILE:CG1	1:B:192:THR:HG23	2.45	0.46	
1:B:494:ALA:O	1:B:498:GLY:O	2.34	0.46	
1:A:374:VAL:HG12	1:A:374:VAL:O	2.16	0.45	
1:A:421:LYS:HB3	1:A:421:LYS:HE2	1.71	0.45	
1:B:123:ARG:NH1	1:B:127:GLU:OE2	2.47	0.45	
1:B:609:SER:OG	1:B:611:GLU:HG2	2.16	0.45	
1:A:141:TYR:CE1	1:A:570:ARG:HG3	2.52	0.45	
1:A:257:TYR:HE1	1:A:281:LEU:HG	1.79	0.45	
1:A:23:ARG:HA	1:A:26:THR:HG22	1.98	0.45	
1:A:174:SER:C	1:A:175:LYS:HG3	2.37	0.45	
1:B:257:TYR:CE1	1:B:281:LEU:HD13	2.51	0.45	
1:A:52:ARG:HG2	1:A:67:TRP:CZ2	2.51	0.45	
1:A:175:LYS:HB3	1:A:178:GLU:CG	2.46	0.45	
1:A:116:LYS:C	1:A:116:LYS:CD	2.85	0.45	
1:A:531:LYS:N	1:A:531:LYS:HD3	2.31	0.45	
1:A:271:VAL:HG11	1:B:356:TYR:CZ	2.51	0.45	
1:B:20:GLU:O	1:B:24:LEU:HB2	2.16	0.45	
1:B:29:LYS:C	1:B:30:ARG:HG2	2.36	0.45	
1:A:76:ASN:HD22	1:A:76:ASN:N	2.15	0.45	
1:A:540:LEU:O	3:A:801:HOH:O	2.21	0.45	
1:B:3:GLU:O	1:B:7:ARG:HB2	2.17	0.45	
1:A:40:ILE:CG2	1:A:44:PHE:CE1	2.98	0.45	



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:40:ILE:HD12	1:B:40:ILE:N	2.32	0.45
1:B:161:LYS:HE3	1:B:161:LYS:HB3	1.85	0.45
1:B:611:GLU:O	1:B:612:GLU:CB	2.64	0.45
1:A:104:GLY:HA2	1:A:107:ILE:HG22	1.99	0.45
1:A:583:LEU:HD23	1:A:583:LEU:HA	1.80	0.45
1:B:157:GLU:HG2	1:B:158:GLN:N	2.19	0.45
1:B:429:ARG:HD3	1:B:477:ARG:NH1	2.27	0.45
1:A:172:ILE:HD11	1:A:177:GLU:OE2	2.17	0.45
1:B:40:ILE:O	1:B:40:ILE:HG22	2.16	0.45
1:B:344:LEU:HG	1:B:599:THR:OG1	2.17	0.45
1:B:102:ILE:HD11	1:B:159:ALA:HA	1.99	0.44
1:B:110:GLY:HA2	1:B:115:VAL:HG11	1.99	0.44
1:B:164:GLU:O	1:B:168:ASP:HB2	2.17	0.44
1:B:236:LYS:H	1:B:236:LYS:CD	2.30	0.44
1:B:370:VAL:HG13	1:B:370:VAL:O	2.18	0.44
1:A:627:MET:HB3	1:A:627:MET:HE2	1.66	0.44
1:B:433:MET:CE	1:B:472:PHE:CE1	3.00	0.44
1:A:148:LEU:HD23	1:A:152:GLU:HG2	1.98	0.44
1:A:227:ASN:OD1	1:A:634:LEU:HD12	2.17	0.44
1:A:612:GLU:C	1:A:614:GLU:H	2.20	0.44
1:B:289:CYS:HB3	1:B:293:ASP:HB3	1.98	0.44
1:B:115:VAL:CG1	1:B:119:LYS:HG3	2.47	0.44
1:B:146:LEU:HD21	1:B:184:VAL:HG22	1.99	0.44
1:B:439:LEU:HD21	1:B:450:LEU:HD13	1.99	0.44
1:A:111:LYS:HD3	1:A:111:LYS:N	2.33	0.44
1:B:174:SER:O	1:B:175:LYS:CG	2.66	0.44
1:B:56:TYR:C	1:B:58:ALA:N	2.71	0.44
1:B:57:MET:HE2	1:B:57:MET:HB3	1.66	0.44
1:B:286:GLU:OE1	1:B:286:GLU:HA	2.16	0.44
1:A:109:PHE:HE1	1:A:111:LYS:HB2	1.82	0.43
1:A:501:ILE:HD13	1:A:501:ILE:H	1.83	0.43
1:A:175:LYS:CB	1:A:178:GLU:HG2	2.45	0.43
1:A:290:GLN:O	1:A:293:ASP:HB2	2.17	0.43
1:B:6:TRP:CH2	1:B:42:LYS:HD3	2.53	0.43
1:B:196:ASN:C	1:B:196:ASN:ND2	2.69	0.43
1:A:109:PHE:HE1	1:A:111:LYS:HG2	1.84	0.43
1:B:56:TYR:C	1:B:58:ALA:H	2.21	0.43
1:A:166:ILE:HG13	1:A:167:ARG:N	2.33	0.43
1:A:611:GLU:O	1:A:614:GLU:HG2	2.19	0.43
1:B:439:LEU:HD23	1:B:439:LEU:O	2.18	0.43
1:A:125:ILE:HG21	1:A:142:ILE:HG21	1.99	0.43



	, and pagein	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:42:LYS:C	1:A:42:LYS:CD	2.87	0.43
1:A:187:ILE:HD13	1:A:187:ILE:N	2.34	0.43
1:A:606:TRP:C	1:A:607:ILE:HG12	2.39	0.43
1:B:363:LEU:HD11	1:B:559:ILE:HD11	2.01	0.43
1:A:30:ARG:O	1:A:30:ARG:HG2	2.18	0.43
1:A:499:ASN:OD1	1:A:501:ILE:HG12	2.18	0.43
1:B:130:LEU:O	1:B:576:LYS:HE3	2.19	0.43
1:B:348:LYS:HE2	1:B:348:LYS:HB3	1.84	0.43
1:B:366:GLY:HA3	1:B:604:PRO:O	2.19	0.43
1:A:516:ASP:O	1:A:519:SER:OG	2.33	0.43
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.75	0.43
1:A:195:LEU:HD23	1:A:199:LYS:HB2	2.01	0.42
1:A:511:LEU:HD23	1:A:511:LEU:HA	1.78	0.42
1:A:482:VAL:HG22	1:A:506:ALA:O	2.19	0.42
1:B:17:ASN:O	1:B:21:ALA:N	2.42	0.42
1:B:430:LEU:HD13	1:B:430:LEU:O	2.19	0.42
1:A:102:ILE:HG12	1:A:163:TYR:HB2	2.01	0.42
1:A:521:LEU:N	1:A:521:LEU:HD22	2.34	0.42
1:B:283:ASP:OD1	1:B:283:ASP:O	2.37	0.42
1:B:563:LEU:HB3	1:B:564:PRO:CD	2.48	0.42
1:A:452:LEU:CB	1:A:453:PRO:HD3	2.49	0.42
1:A:521:LEU:HA	1:A:525:GLU:OE2	2.19	0.42
1:B:515:MET:HG2	1:B:518:VAL:CG1	2.48	0.42
1:B:515:MET:HE1	1:B:518:VAL:HG13	2.01	0.42
1:A:504:THR:HG23	1:A:530:ILE:CD1	2.50	0.42
1:A:626:TRP:HA	1:A:631:GLN:HG2	2.01	0.42
1:B:73:ILE:O	1:B:73:ILE:CG2	2.51	0.42
1:B:107:ILE:HD13	1:B:107:ILE:HG21	1.81	0.42
1:B:466:LEU:O	1:B:470:VAL:HG23	2.20	0.42
1:A:110:GLY:CA	1:A:115:VAL:HG11	2.47	0.42
1:B:461:GLN:O	1:B:464:SER:OG	2.35	0.42
1:A:572:ILE:HG21	1:A:575:LEU:HG	2.01	0.42
1:B:115:VAL:HG12	1:B:119:LYS:HG3	2.02	0.42
1:A:130:LEU:O	1:A:576:LYS:HG3	2.20	0.42
1:A:161:LYS:NZ	1:A:162:LEU:HD12	2.35	0.42
1:A:161:LYS:HD2	1:A:161:LYS:C	2.40	0.42
1:B:17:ASN:HB3	1:B:20:GLU:OE1	2.19	0.42
1:B:461:GLN:HA	1:B:464:SER:HG	1.84	0.42
1:A:23:ARG:O	1:A:26:THR:HG23	2.17	0.42
1:B:40:ILE:O	1:B:40:ILE:CG2	2.68	0.42
1:B:52:ARG:CZ	1:B:80:LEU:HD11	2.50	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:611:GLU:O	1:B:612:GLU:HB2	2.19	0.42
1:B:283:ASP:O	1:B:285:ASP:N	2.53	0.41
2:B:701:UPG:H3'	2:B:701:UPG:H5C2	2.02	0.41
1:B:74:LEU:HD22	1:B:77:ILE:HD11	2.01	0.41
1:B:125:ILE:O	1:B:129:ILE:HB	2.20	0.41
1:B:512:VAL:O	1:B:512:VAL:HG23	2.20	0.41
1:A:23:ARG:NE	1:A:61:PHE:CZ	2.88	0.41
1:B:29:LYS:O	1:B:30:ARG:CD	2.63	0.41
1:B:24:LEU:HD22	1:B:24:LEU:HA	1.83	0.41
1:B:130:LEU:C	1:B:576:LYS:HG3	2.40	0.41
1:B:515:MET:HE1	1:B:518:VAL:CG2	2.50	0.41
1:B:541:LEU:HA	1:B:541:LEU:HD23	1.75	0.41
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.74	0.41
1:A:359:HIS:ND1	1:A:360:PRO:HD2	2.35	0.41
1:A:512:VAL:O	1:A:512:VAL:CG2	2.69	0.41
1:B:114:VAL:HG21	1:B:166:ILE:HA	2.01	0.41
1:B:348:LYS:O	1:B:348:LYS:HG2	2.21	0.41
1:A:284:PHE:CE2	1:A:301:GLN:NE2	2.88	0.41
1:B:113:PRO:HG2	1:B:170:LYS:O	2.21	0.41
1:B:543:LYS:N	1:B:544:PRO:HD2	2.35	0.41
1:B:158:GLN:O	1:B:162:LEU:HB2	2.20	0.41
1:A:23:ARG:HA	1:A:26:THR:CG2	2.51	0.41
1:A:40:ILE:N	1:A:40:ILE:CD1	2.83	0.41
1:B:119:LYS:HG2	1:B:143:PHE:CD1	2.56	0.41
1:B:133:GLU:HA	1:B:134:PRO:HD2	1.82	0.41
1:B:162:LEU:HD12	1:B:162:LEU:C	2.41	0.41
1:B:439:LEU:HD23	1:B:439:LEU:C	2.40	0.41
1:B:512:VAL:O	1:B:512:VAL:CG2	2.69	0.41
1:B:522:ASN:CG	1:B:525:GLU:HB2	2.41	0.41
1:A:74:LEU:C	1:A:76:ASN:N	2.75	0.40
1:A:129:ILE:HD12	1:A:129:ILE:HA	1.69	0.40
1:A:512:VAL:O	1:A:512:VAL:HG23	2.20	0.40
1:B:44:PHE:HD1	1:B:44:PHE:H	0.69	0.40
1:A:110:GLY:HA2	1:A:115:VAL:CG1	2.49	0.40
1:A:442:ASP:O	1:A:446:ASN:CB	2.65	0.40
1:A:509:ALA:O	1:A:512:VAL:O	2.39	0.40
1:A:563:LEU:HA	1:A:564:PRO:HD3	1.83	0.40
1:B:29:LYS:CE	1:B:42:LYS:HE2	2.44	0.40
1:B:45:GLU:H	1:B:45:GLU:HG2	1.70	0.40
1:B:439:LEU:CD2	1:B:450:LEU:HD13	2.52	0.40
1:B:567:GLU:HA	1:B:568:PRO:HD3	1.73	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:THR:HG23	1:A:13:GLU:HG3	2.04	0.40
1:A:266:GLU:OE1	1:A:266:GLU:HA	2.21	0.40
1:B:157:GLU:HA	1:B:160:GLU:HG3	2.04	0.40
1:B:167:ARG:HG3	1:B:168:ASP:OD2	2.22	0.40
1:A:17:ASN:O	1:A:21:ALA:HB3	2.20	0.40
1:B:254:LYS:HD2	1:B:282:LEU:HD12	2.04	0.40
1:B:273:TRP:CH2	1:B:279:ILE:HD13	2.57	0.40
1:B:532:LYS:HE2	1:B:532:LYS:HB2	1.95	0.40
1:B:567:GLU:CG	1:B:568:PRO:CD	2.91	0.40
1:B:140:GLU:CG	1:B:374:VAL:HG23	2.35	0.40
1:B:195:LEU:HD22	1:B:199:LYS:HB3	2.03	0.40
1:B:525:GLU:O	1:B:529:LEU:N	2.55	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	Perce	entiles
1	А	599/655~(92%)	561 (94%)	33~(6%)	5 (1%)	19	29
1	В	583/655~(89%)	543 (93%)	35~(6%)	5 (1%)	17	25
All	All	1182/1310 (90%)	1104 (93%)	68~(6%)	10 (1%)	19	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	41	ASN
1	А	249	ALA
1	В	249	ALA
1	В	565	THR
1	В	519	SER
1	В	57	MET



Continued from previous page...

Mol	Chain	Res	Type
1	В	284	PHE
1	А	30	ARG
1	А	566	GLY
1	А	613	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Per	$\operatorname{centiles}$
1	А	533/578~(92%)	479 (90%)	54 (10%)	7	11
1	В	519/578~(90%)	471 (91%)	48 (9%)	9	13
All	All	1052/1156~(91%)	950~(90%)	102 (10%)	8	12

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	3	GLU
1	А	5	TYR
1	А	10	LEU
1	А	23	ARG
1	А	24	LEU
1	А	38	GLU
1	А	40	ILE
1	А	41	ASN
1	А	42	LYS
1	А	46	ASN
1	А	52	ARG
1	А	54	SER
1	А	73	ILE
1	А	81	THR
1	А	109	PHE
1	А	111	LYS
1	А	119	LYS
1	А	129	ILE
1	А	146	LEU



Mol	Chain	Res	Type
1	А	161	LYS
1	А	162	LEU
1	А	165	CYS
1	А	166	ILE
1	А	167	ARG
1	А	169	LYS
1	А	170	LYS
1	А	175	LYS
1	А	180	LEU
1	А	284	PHE
1	А	352	SER
1	А	407	SER
1	А	441	LYS
1	А	444	GLU
1	А	449	LYS
1	А	461	GLN
1	А	467	SER
1	А	471	ARG
1	А	476	GLN
1	А	482	VAL
1	А	501	ILE
1	А	502	VAL
1	А	513	HIS
1	А	515	MET
1	А	522	ASN
1	А	531	LYS
1	А	539	SER
1	А	543	LYS
1	А	596	THR
1	А	609	SER
1	А	611	GLU
1	А	614	GLU
1	А	615	ARG
1	А	624	LEU
1	А	634	LEU
1	В	12	THR
1	В	13	GLU
1	В	23	ARG
1	В	24	LEU
1	В	30	ARG
1	В	39	SER
1	В	42	LYS



Mol	Chain	Res	Type
1	В	44	PHE
1	В	46	ASN
1	В	52	ARG
1	В	107	ILE
1	В	112	SER
1	В	114	VAL
1	В	123	ARG
1	В	129	ILE
1	В	133	GLU
1	В	135	ASN
1	В	158	GLN
1	В	162	LEU
1	В	169	LYS
1	В	178	GLU
1	В	186	ARG
1	В	196	ASN
1	В	235	LYS
1	В	236	LYS
1	В	345	THR
1	В	349	SER
1	В	371	LYS
1	В	374	VAL
1	В	420	SER
1	В	475	VAL
1	В	496	GLN
1	В	507	LEU
1	В	511	LEU
1	В	515	MET
1	В	516	ASP
1	В	518	VAL
1	В	520	ARG
1	В	522	ASN
1	В	524	SER
1	В	525	GLU
1	В	529	LEU
1	В	543	LYS
1	В	546	VAL
1	В	599	THR
1	В	608	THR
1	В	624	LEU
1	В	629	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)



such sidechains are listed below:

Mol	Chain	Res	Type
1	А	46	ASN
1	А	76	ASN
1	А	120	GLN
1	А	121	ASN
1	А	492	GLN
1	А	513	HIS
1	В	17	ASN
1	В	46	ASN
1	В	121	ASN
1	В	135	ASN
1	В	138	GLN
1	В	196	ASN
1	В	248	ASN
1	В	446	ASN
1	В	492	GLN
1	В	513	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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).



Mal Turna C		Chain Dec		Tink	Bo	ond leng	$_{\rm ths}$	E	Bond ang	gles
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	UPG	В	701	-	35,38,38	1.12	2 (5%)	$53,\!58,\!58$	2.14	12 (22%)
2	UPG	А	701	-	35,38,38	1.18	6 (17%)	53,58,58	2.12	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UPG	В	701	-	-	1/23/59/59	0/3/3/3
2	UPG	А	701	-	-	3/23/59/59	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
2	В	701	UPG	C6-N1	-2.54	1.31	1.38
2	А	701	UPG	C2-N1	2.36	1.42	1.38
2	А	701	UPG	C6-N1	-2.34	1.32	1.38
2	В	701	UPG	PB-O2B	-2.33	1.44	1.55
2	А	701	UPG	PB-O2B	-2.30	1.44	1.55
2	А	701	UPG	PB-O1B	-2.13	1.43	1.50
2	А	701	UPG	PA-O1A	-2.13	1.43	1.50
2	А	701	UPG	O4C-C4C	-2.10	1.40	1.45

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	701	UPG	O2-C2-N1	-7.59	112.70	122.79
2	А	701	UPG	O2-C2-N1	-7.09	113.36	122.79
2	А	701	UPG	C4-N3-C2	-6.40	118.14	126.58
2	В	701	UPG	C4-N3-C2	-6.07	118.57	126.58
2	В	701	UPG	N3-C2-N1	6.05	122.93	114.89
2	А	701	UPG	N3-C2-N1	5.60	122.33	114.89
2	А	701	UPG	O4-C4-C5	-4.23	117.72	125.16
2	В	701	UPG	O4-C4-C5	-4.21	117.75	125.16
2	А	701	UPG	O5'-C1'-O3B	-4.06	106.06	111.36
2	В	701	UPG	O4-C4-N3	3.12	123.89	119.31
2	А	701	UPG	O4-C4-N3	2.77	123.37	119.31
2	А	701	UPG	C5-C4-N3	2.71	118.90	114.84
2	В	701	UPG	C6-N1-C2	-2.71	117.52	120.99
2	В	701	UPG	O4C-C1C-N1	2.67	114.46	108.36



Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	В	701	UPG	C1'-O5'-C5'	2.36	118.31	113.69
2	В	701	UPG	C5-C4-N3	2.35	118.36	114.84
2	В	701	UPG	C1C-N1-C2	2.31	121.74	117.57
2	В	701	UPG	O2B-PB-O1B	2.22	123.23	112.24
2	В	701	UPG	O5C-PA-O1A	-2.14	100.69	109.07
2	А	701	UPG	C1'-O5'-C5'	2.04	117.69	113.69

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	А	701	UPG	PB-O3A-PA-O1A
2	А	701	UPG	O5'-C1'-O3B-PB
2	А	701	UPG	PB-O3A-PA-O2A
2	В	701	UPG	C1'-O3B-PB-O3A

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	701	UPG	1	0
2	А	701	UPG	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 then 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, 95^{th} 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	0	$\mathbf{DWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	607/655~(92%)	0.48	28 (4%) 32 31	38	8, 63, 96, 120	0
1	В	591/655~(90%)	0.53	34 (5%) 23 22	37	7, 60, 97, 109	0
All	All	1198/1310~(91%)	0.50	62 (5%) 27 26	37	7, 62, 97, 120	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	521	LEU	6.2
1	А	345	THR	5.4
1	В	44	PHE	5.4
1	А	619	LEU	5.0
1	В	114	VAL	4.4
1	А	5	TYR	4.3
1	А	109	PHE	4.2
1	А	615	ARG	4.1
1	В	166	ILE	3.9
1	А	617	GLN	3.8
1	А	634	LEU	3.6
1	А	44	PHE	3.6
1	А	81	THR	3.5
1	В	525	GLU	3.4
1	А	29	LYS	3.4
1	В	162	LEU	3.3
1	В	515	MET	3.1
1	В	163	TYR	3.1
1	А	445	GLU	3.0
1	А	111	LYS	3.0
1	В	10	LEU	3.0
1	В	264	LYS	2.8
1	В	46	ASN	2.8
1	A	79	PRO	2.7



Mol	Chain	Res	Type	RSRZ	
1	В	345	THR	2.7	
1	В	495	LEU	2.7	
1	В	130	LEU	2.7	
1	В	174	SER	2.6	
1	А	616	THR	2.6	
1	В	167	ARG	2.6	
1	А	41	ASN	2.6	
1	В	175	LYS	2.6	
1	В	24	LEU	2.6	
1	А	78	GLN	2.5	
1	А	482	VAL	2.5	
1	В	624	LEU	2.5	
1	В	159	ALA	2.4	
1	А	344	LEU	2.4	
1	В	117	LEU	2.4	
1	А	142	ILE	2.4	
1	А	67	TRP	2.3	
1	В	598	PHE	2.3	
1	В	176	PHE	2.3	
1	А	623	GLY	2.3	
1	В	491	PHE	2.3	
1	В	7	ARG	2.3	
1	В	567	GLU	2.3	
1	А	630	GLU	2.3	
1	В	518	VAL	2.2	
1	А	76	ASN	2.2	
1	В	507	LEU	2.2	
1	А	187	ILE	2.2	
1	В	4	GLN	2.2	
1	В	520	ARG	2.1	
1	А	77	ILE	2.1	
1	А	40	ILE	2.1	
1	В	529	LEU	2.1	
1	А	18	GLN	2.1	
1	В	446	ASN	2.1	
1	В	47	ASP	2.0	
1	В	8	PHE	2.0	
1	А	162	LEU	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 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
2	UPG	В	701	36/36	0.93	0.18	44,61,73,77	0
2	UPG	А	701	36/36	0.94	0.20	41,62,76,79	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 (i)

There are no such residues in this entry.

