

Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2021 – 08:26 PM EDT

PDB ID	:	1S9E
Title	:	CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE (RT) IN
		COMPLEX WITH JANSSEN-R129385
Authors	:	Das, K.; Clark Jr., A.D.; Ludovici, D.W.; Kukla, M.J.; Decorte, B.; Lewi, P.J.;
		Hughes, S.H.; Janssen, P.A.; Arnold, E.
Deposited on	:	2004-02-04
Resolution	:	2.60 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 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	:	2.23.2
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)	:	2.23.2

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 2.60 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.



Motria	Whole archive	Similar resolution
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	560	3%	54%	10%
2	В	430	33%	54%	12% ••



 $\mathbf{2}$

Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8231 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 POL polyprotein [Contains:Reverse transcriptase].

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	552	Total 4498	C 2913	N 748	O 830	${ m S} 7$	122	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	280	SER	CYS	engineered mutation	UNP P03366

• Molecule 2 is a protein called POL polyprotein [Contains: Reverse transcriptase].

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
2	В	427	Total 3529	C 2300	N 584	O 638	S 7	56	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366

• Molecule 3 is 4-[4-AMINO-6-(2,6-DICHLORO-PHENOXY)-[1,3,5]TRIAZIN-2-YLAMINO]-BENZONITRILE (three-letter code: ADB) (formula: C₁₆H₁₀Cl₂N₆O).







Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
3	Δ	1	Total	С	Cl	Ν	0	0	0
0	11	I	25	16	2	6	1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	85	Total O 85 85	0	0
4	В	94	Total O 94 94	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: POL polyprotein [Contains:Reverse transcriptase]



• Molecule 2: POL polyprotein [Contains: Reverse transcriptase]

Chain B:

33%

54%

12% •









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	226.80Å 69.30Å 104.10Å	Depositor
a, b, c, α , β , γ	90.00° 106.70° 90.00°	Depositor
Bosolution(A)	20.00 - 2.60	Depositor
Resolution (A)	34.69 - 2.60	EDS
% Data completeness	93.3 (20.00-2.60)	Depositor
(in resolution range)	95.8 (34.69-2.60)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.92 (at 2.61 \text{\AA})$	Xtriage
Refinement program	CNS 1.0	Depositor
P. P.	0.253 , 0.316	Depositor
n, n_{free}	0.248 , 0.306	DCC
R_{free} test set	2293 reflections $(4.99%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	56.5	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 70.7	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8231	wwPDB-VP
Average B, all atoms $(Å^2)$	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.33% 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: ADB

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	Bo	nd lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.67	0/4616	0.89	4/6271~(0.1%)	
2	В	0.78	1/3634~(0.0%)	0.95	5/4940~(0.1%)	
All	All	0.72	1/8250~(0.0%)	0.92	9/11211~(0.1%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	383	TRP	CB-CG	-5.55	1.40	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	7	THR	N-CA-C	8.01	132.63	111.00
1	А	381	VAL	CB-CA-C	-6.29	99.46	111.40
1	А	56	TYR	N-CA-C	-6.16	94.36	111.00
1	А	333	GLY	N-CA-C	5.61	127.12	113.10
2	В	78	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	В	89	GLU	N-CA-C	-5.56	95.98	111.00
1	А	135	ILE	N-CA-C	5.53	125.92	111.00
2	В	12	LEU	CA-CB-CG	5.39	127.71	115.30
2	В	155	GLY	N-CA-C	-5.11	100.33	113.10



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
2	В	130	PHE	Sidechain
2	В	144	TYR	Sidechain
2	В	318	TYR	Sidechain

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	4498	0	4560	481	0
2	В	3529	0	3568	378	0
3	А	25	0	10	4	0
4	А	85	0	0	4	0
4	В	94	0	0	17	0
All	All	8231	0	8138	836	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 53.

All (836) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:A:244:ILE:HD11	1:A:310:LEU:HD13	1.26	1.14
1:A:435:VAL:HG13	2:B:290:THR:HG21	1.31	1.09
2:B:278:GLN:HA	2:B:281:LYS:HE3	1.30	1.09
1:A:224:GLU:HB3	1:A:225:PRO:HD2	1.38	1.04
1:A:497:THR:HG22	1:A:499:SER:H	1.21	1.04
2:B:362:THR:HG22	2:B:367:GLN:HE21	1.16	1.04
2:B:277:ARG:H	2:B:277:ARG:HD3	1.18	1.03
2:B:363:ASN:C	2:B:363:ASN:HD22	1.63	1.01
2:B:363:ASN:ND2	2:B:366:LYS:H	1.59	1.00
1:A:288:ALA:CB	1:A:291:GLU:HB2	1.91	0.98
2:B:5:ILE:HG22	2:B:6:GLU:H	1.29	0.98
2:B:65:LYS:HA	2:B:72:ARG:HG3	1.46	0.97
2:B:221:HIS:CE1	2:B:230:MET:HG2	2.01	0.95



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.45	0.95
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.05	0.94
1:A:328:GLU:HG3	1:A:390:LYS:HB2	1.50	0.94
1:A:22:LYS:HG2	1:A:24:TRP:CZ2	2.03	0.94
2:B:363:ASN:HD21	2:B:366:LYS:H	1.02	0.93
2:B:282:LEU:HG	2:B:293:ILE:HD11	1.47	0.92
1:A:503:LEU:HG	1:A:507:GLN:NE2	1.85	0.92
1:A:460:ASN:N	1:A:460:ASN:HD22	1.66	0.91
2:B:274:ILE:HG23	2:B:306:ASN:OD1	1.70	0.91
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.53	0.90
1:A:542:ILE:HD13	1:A:544:GLY:H	1.36	0.90
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.35	0.90
1:A:79:GLU:HG3	1:A:83:ARG:HH12	1.37	0.90
1:A:96:HIS:HD2	1:A:98:ALA:H	1.17	0.89
1:A:122:GLU:HA	1:A:125:ARG:HD2	1.53	0.89
2:B:85:GLN:HG3	2:B:154:LYS:CB	2.02	0.89
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.56	0.88
2:B:362:THR:CG2	2:B:367:GLN:HE21	1.87	0.88
1:A:506:ILE:HG21	1:A:533:LEU:HD12	1.54	0.87
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.58	0.86
2:B:303:LEU:O	2:B:307:ARG:HB2	1.75	0.86
2:B:310:LEU:O	2:B:310:LEU:HD23	1.76	0.86
1:A:90:VAL:HG12	1:A:91:GLN:HG3	1.57	0.86
1:A:226:PRO:HG3	1:A:235:HIS:CE1	2.11	0.86
1:A:465:LYS:HG3	1:A:466:VAL:N	1.88	0.86
2:B:278:GLN:NE2	2:B:298:GLU:HB2	1.91	0.86
2:B:363:ASN:HD21	2:B:366:LYS:N	1.73	0.85
2:B:31:ILE:O	2:B:35:VAL:HG23	1.75	0.85
1:A:406:TRP:CZ3	2:B:420:PRO:HD2	2.10	0.85
1:A:388:LYS:NZ	1:A:413:GLU:HG3	1.92	0.85
2:B:244:ILE:O	2:B:310:LEU:HD21	1.76	0.85
1:A:104:LYS:HE2	1:A:104:LYS:N	1.92	0.84
1:A:460:ASN:HD22	1:A:460:ASN:H	1.25	0.84
1:A:497:THR:HG22	1:A:498:ASP:N	1.89	0.84
1:A:148:VAL:O	1:A:150:PRO:HD3	1.77	0.84
2:B:104:LYS:HA	2:B:237:ASP:OD2	1.77	0.84
2:B:257:ILE:HG23	2:B:283:LEU:HD21	1.59	0.84
1:A:224:GLU:HB3	1:A:225:PRO:CD	2.07	0.84
1:A:254:VAL:O	1:A:257:ILE:HG22	1.78	0.84
1:A:542:ILE:HG12	1:A:543:GLY:H	1.43	0.83
2:B:422:LEU:HD12	2:B:425:LEU:HD12	1.61	0.83



	lo ao pagom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:104:LYS:HG2	1:A:192:ASP:HA	1.61	0.82
1:A:435:VAL:CG1	2:B:290:THR:HG21	2.07	0.82
1:A:442:VAL:HG13	1:A:481:ALA:HB1	1.59	0.81
1:A:96:HIS:CD2	1:A:98:ALA:H	1.99	0.81
2:B:345:PRO:HB2	2:B:346:PHE:CD1	2.15	0.81
1:A:46:LYS:HD3	1:A:116:PHE:HB3	1.62	0.81
1:A:64:LYS:HE3	1:A:68:SER:HB3	1.62	0.81
1:A:97:PRO:HG2	1:A:232:TYR:CD2	2.15	0.81
2:B:249:LYS:HD2	2:B:252:TRP:CZ3	2.16	0.81
1:A:155:GLY:O	1:A:159:ILE:HG13	1.81	0.80
2:B:206:ARG:HB3	2:B:206:ARG:NH1	1.96	0.80
1:A:337:TRP:HE1	1:A:367:GLN:NE2	1.80	0.80
2:B:296:THR:OG1	2:B:299:ALA:HB2	1.83	0.79
2:B:85:GLN:HG3	2:B:154:LYS:HB3	1.65	0.79
2:B:85:GLN:HG2	4:B:1089:HOH:O	1.81	0.79
1:A:206:ARG:HH22	1:A:217:PRO:C	1.86	0.78
1:A:224:GLU:CB	1:A:225:PRO:HD2	2.11	0.78
1:A:136:ASN:O	1:A:138:GLU:N	2.16	0.78
1:A:298:GLU:H	1:A:298:GLU:CD	1.87	0.78
1:A:53:GLU:C	1:A:55:PRO:HD3	2.03	0.77
1:A:287:LYS:HG2	1:A:288:ALA:H	1.49	0.77
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.67	0.77
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.15	0.77
1:A:138:GLU:HA	1:A:138:GLU:OE2	1.85	0.77
1:A:220:LYS:HB2	4:A:1009:HOH:O	1.85	0.77
1:A:540:LYS:HD2	2:B:265:ASN:ND2	2.00	0.77
2:B:369:THR:HG22	2:B:373:GLN:HE21	1.50	0.76
1:A:115:TYR:HD2	1:A:149:LEU:O	1.69	0.76
1:A:315:HIS:CE1	1:A:347:LYS:HD3	2.20	0.76
1:A:19:PRO:HG3	1:A:80:LEU:HA	1.66	0.76
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.21	0.76
1:A:139:THR:HB	1:A:140:PRO:HD2	1.66	0.76
1:A:506:ILE:HG21	1:A:533:LEU:CD1	2.15	0.76
2:B:366:LYS:HG3	2:B:405:TYR:CD2	2.21	0.75
1:A:181:TYR:HE2	1:A:183:TYR:HB2	1.50	0.75
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.68	0.75
1:A:506:ILE:HG22	1:A:507:GLN:N	2.00	0.75
2:B:222:GLN:HG2	2:B:223:LYS:HG2	1.68	0.75
1:A:97:PRO:HG2	1:A:232:TYR:CE2	2.22	0.75
1:A:287:LYS:H	1:A:287:LYS:HD3	1.51	0.75
1:A:1:PRO:0	1:A:117:SER:HA	1.87	0.75



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:10:VAL:HG12	1:A:11:LYS:N	2.02	0.74
2:B:366:LYS:HG3	2:B:405:TYR:CG	2.22	0.74
2:B:298:GLU:HB3	2:B:301:LEU:HD13	1.69	0.74
1:A:183:TYR:CE2	1:A:230:MET:SD	2.81	0.74
1:A:503:LEU:HG	1:A:507:GLN:HE22	1.51	0.74
1:A:509:GLN:N	1:A:510:PRO:HD3	2.02	0.74
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.23	0.74
1:A:96:HIS:HD2	1:A:98:ALA:N	1.85	0.74
1:A:497:THR:HG22	1:A:499:SER:N	2.01	0.74
1:A:58:THR:HG22	1:A:59:PRO:HD2	1.68	0.74
1:A:417:VAL:HG12	1:A:419:THR:HG23	1.68	0.74
1:A:388:LYS:HZ2	1:A:413:GLU:HG3	1.52	0.73
1:A:312:GLU:O	1:A:312:GLU:HG2	1.89	0.73
2:B:356:ARG:HG2	2:B:362:THR:HG21	1.69	0.73
1:A:540:LYS:HD2	2:B:265:ASN:HD21	1.52	0.73
2:B:356:ARG:HG3	2:B:357:MET:H	1.52	0.73
2:B:257:ILE:CG2	2:B:283:LEU:HD21	2.18	0.73
2:B:27:THR:CG2	2:B:29:GLU:HB3	2.19	0.73
1:A:28:GLU:HB3	1:A:135:ILE:HD13	1.71	0.73
1:A:232:TYR:OH	1:A:269:GLN:NE2	2.22	0.73
1:A:382:ILE:HG23	2:B:136:ASN:ND2	2.04	0.73
1:A:542:ILE:HG12	1:A:543:GLY:N	2.04	0.73
1:A:438:GLU:HG3	1:A:460:ASN:HD21	1.54	0.72
2:B:85:GLN:HG3	2:B:154:LYS:HB2	1.70	0.72
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.71	0.72
2:B:278:GLN:HE22	2:B:298:GLU:HB2	1.53	0.72
2:B:373:GLN:HE22	2:B:406:TRP:HA	1.55	0.72
1:A:435:VAL:HG13	2:B:290:THR:CG2	2.14	0.72
1:A:55:PRO:HD2	1:A:143:ARG:HH12	1.55	0.71
2:B:362:THR:HG22	2:B:367:GLN:NE2	2.00	0.71
1:A:253:THR:OG1	1:A:290:THR:HA	1.90	0.71
1:A:64:LYS:HE3	1:A:68:SER:CB	2.21	0.71
1:A:424:LYS:HD3	1:A:425:LEU:N	2.05	0.71
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.31	0.71
2:B:278:GLN:OE1	2:B:297:GLU:HB2	1.90	0.71
1:A:503:LEU:CD2	1:A:535:TRP:HB2	2.20	0.71
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.26	0.71
2:B:345:PRO:HB2	2:B:346:PHE:HD1	1.54	0.71
1:A:301:LEU:O	1:A:305:GLU:HG3	1.90	0.70
2:B:221:HIS:HE1	2:B:230:MET:HG2	1.55	0.70
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.26	0.70



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:542:ILE:HD13	1:A:544:GLY:N	2.06	0.70
1:A:30:LYS:HD3	1:A:62:ALA:HB3	1.74	0.70
1:A:30:LYS:O	1:A:33:ALA:N	2.25	0.70
1:A:507:GLN:O	1:A:509:GLN:HG3	1.91	0.70
2:B:278:GLN:HA	2:B:281:LYS:CE	2.18	0.70
1:A:373:GLN:OE1	2:B:397:THR:HA	1.91	0.70
1:A:495:ILE:HB	1:A:533:LEU:HD23	1.74	0.70
2:B:298:GLU:HB3	2:B:301:LEU:CD1	2.22	0.69
2:B:418:ASN:O	2:B:419:THR:HG23	1.92	0.69
1:A:33:ALA:O	1:A:37:ILE:HG12	1.92	0.69
1:A:103:LYS:C	1:A:104:LYS:HE2	2.12	0.69
1:A:277:ARG:HD2	1:A:334:GLN:CB	2.23	0.69
1:A:497:THR:CG2	1:A:499:SER:H	2.03	0.69
1:A:277:ARG:HD2	1:A:334:GLN:HB3	1.75	0.68
1:A:7:THR:HG22	1:A:119:PRO:HB2	1.74	0.68
1:A:27:THR:O	1:A:29:GLU:N	2.25	0.68
1:A:518:VAL:O	1:A:522:ILE:HG13	1.94	0.68
1:A:376:THR:HG23	1:A:386:THR:HG22	1.75	0.68
2:B:371:ALA:O	2:B:375:ILE:HG13	1.93	0.68
1:A:331:LYS:NZ	1:A:333:GLY:HA2	2.09	0.68
1:A:373:GLN:HG2	2:B:394:GLN:NE2	2.09	0.68
2:B:277:ARG:HD3	2:B:277:ARG:N	2.00	0.68
1:A:398:TRP:NE1	1:A:402:TRP:HD1	1.92	0.68
1:A:162:SER:HB2	2:B:52:PRO:HG3	1.74	0.68
1:A:474:ASN:O	1:A:478:GLU:HG3	1.95	0.67
1:A:286:THR:O	1:A:286:THR:HG22	1.93	0.67
1:A:244:ILE:HD11	1:A:310:LEU:CD1	2.15	0.67
1:A:326:ILE:HD12	1:A:326:ILE:N	2.09	0.67
2:B:357:MET:HB2	2:B:361:HIS:HE2	1.59	0.67
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.20	0.67
1:A:354:TYR:OH	1:A:356:ARG:HD3	1.94	0.67
2:B:101:LYS:O	2:B:236:PRO:HB2	1.95	0.67
2:B:388:LYS:HE3	2:B:415:GLU:OE1	1.95	0.67
1:A:542:ILE:CD1	1:A:544:GLY:H	2.07	0.67
1:A:29:GLU:OE1	1:A:29:GLU:HA	1.94	0.66
2:B:257:ILE:O	2:B:261:VAL:HG23	1.95	0.66
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.10	0.66
1:A:301:LEU:O	1:A:301:LEU:HD12	1.95	0.66
2:B:357:MET:HB2	2:B:361:HIS:NE2	2.10	0.66
2:B:5:ILE:HG22	2:B:6:GLU:N	2.08	0.66
2:B:278:GLN:HE22	2:B:298:GLU:CB	2.07	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:417:VAL:HG12	1:A:417:VAL:O	1.96	0.66
2:B:86:ASP:O	2:B:89:GLU:HB3	1.95	0.66
1:A:460:ASN:N	1:A:460:ASN:ND2	2.40	0.66
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.32	0.65
1:A:27:THR:O	1:A:30:LYS:N	2.28	0.65
1:A:290:THR:O	1:A:290:THR:HG22	1.96	0.65
1:A:340:GLN:HB3	1:A:351:THR:HG22	1.76	0.65
2:B:23:GLN:HB2	4:B:1090:HOH:O	1.95	0.65
2:B:278:GLN:HE22	2:B:298:GLU:CG	2.09	0.65
2:B:422:LEU:O	2:B:425:LEU:HB2	1.96	0.65
1:A:10:VAL:HG12	1:A:11:LYS:H	1.59	0.65
1:A:434:ILE:H	1:A:494:ASN:HD21	1.43	0.65
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.27	0.65
1:A:315:HIS:NE2	1:A:347:LYS:HD3	2.11	0.65
2:B:53:GLU:OE1	2:B:53:GLU:N	2.29	0.65
1:A:225:PRO:HA	1:A:226:PRO:C	2.17	0.65
1:A:298:GLU:CD	1:A:298:GLU:N	2.50	0.64
1:A:363:ASN:OD1	1:A:365:VAL:N	2.30	0.64
1:A:56:TYR:CD1	1:A:56:TYR:N	2.64	0.64
2:B:76:ASP:CG	2:B:78:ARG:HH21	2.00	0.64
2:B:411:ILE:HA	4:B:1088:HOH:O	1.97	0.64
1:A:279:LEU:CD2	1:A:299:ALA:HB1	2.25	0.64
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.62	0.64
2:B:46:LYS:CE	2:B:116:PHE:HD1	2.11	0.64
2:B:339:TYR:C	2:B:340:GLN:OE1	2.36	0.64
2:B:335:GLY:O	2:B:355:ALA:HA	1.97	0.64
2:B:85:GLN:HA	4:B:1089:HOH:O	1.98	0.63
1:A:270:ILE:O	1:A:272:PRO:HD3	1.98	0.63
2:B:156:SER:N	2:B:157:PRO:HD2	2.13	0.63
2:B:46:LYS:HD3	2:B:116:PHE:CD1	2.33	0.63
1:A:433:PRO:HG3	2:B:255:ASN:HD22	1.63	0.63
2:B:278:GLN:NE2	2:B:298:GLU:CB	2.61	0.63
1:A:373:GLN:HG2	2:B:394:GLN:HE22	1.64	0.63
1:A:497:THR:CG2	1:A:498:ASP:N	2.59	0.63
2:B:363:ASN:C	2:B:363:ASN:ND2	2.39	0.63
2:B:359:GLY:O	2:B:361:HIS:N	2.32	0.63
1:A:50:ILE:HG13	1:A:51:GLY:N	2.13	0.63
1:A:420:PRO:HA	1:A:421:PRO:C	2.18	0.62
2:B:195:ILE:HG23	2:B:196:GLY:N	2.13	0.62
2:B:266:TRP:HZ3	2:B:426:TRP:CD1	2.17	0.62
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.00	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:400:THR:O	1:A:403:THR:HB	1.99	0.62
2:B:217:PRO:O	2:B:219:LYS:N	2.32	0.62
2:B:305:GLU:HG3	2:B:306:ASN:N	2.14	0.62
1:A:35:VAL:O	1:A:39:THR:HG23	1.98	0.62
1:A:287:LYS:H	1:A:287:LYS:CD	2.12	0.62
2:B:357:MET:CB	2:B:361:HIS:HE2	2.13	0.62
1:A:27:THR:O	1:A:27:THR:HG22	1.99	0.62
1:A:492:GLU:OE1	1:A:530:LYS:HD2	2.00	0.62
1:A:501:TYR:O	1:A:505:ILE:HD12	1.99	0.62
2:B:282:LEU:CG	2:B:293:ILE:HD11	2.27	0.62
2:B:373:GLN:HG2	2:B:406:TRP:CH2	2.35	0.62
1:A:474:ASN:HD22	1:A:474:ASN:H	1.48	0.62
2:B:267:ALA:HB2	2:B:426:TRP:CH2	2.35	0.62
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.28	0.61
1:A:460:ASN:H	1:A:460:ASN:ND2	1.94	0.61
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.15	0.61
1:A:442:VAL:HG13	1:A:481:ALA:CB	2.30	0.61
2:B:411:ILE:O	2:B:412:PRO:C	2.37	0.61
1:A:10:VAL:CG1	1:A:11:LYS:H	2.14	0.61
2:B:221:HIS:NE2	2:B:230:MET:HG2	2.16	0.61
2:B:224:GLU:O	2:B:226:PRO:HD3	2.00	0.61
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.65	0.61
1:A:398:TRP:CD1	1:A:402:TRP:HD1	2.18	0.61
2:B:87:PHE:O	2:B:91:GLN:HB2	2.00	0.60
2:B:266:TRP:CZ3	2:B:426:TRP:CD1	2.87	0.60
2:B:255:ASN:O	2:B:258:GLN:HB2	2.01	0.60
1:A:90:VAL:HG12	1:A:91:GLN:CG	2.28	0.60
1:A:115:TYR:CD2	1:A:149:LEU:O	2.54	0.60
1:A:388:LYS:HZ3	1:A:413:GLU:HG3	1.66	0.60
2:B:369:THR:O	2:B:373:GLN:HG3	2.00	0.60
1:A:81:ASN:C	1:A:83:ARG:H	2.03	0.60
1:A:102:LYS:HG2	1:A:104:LYS:NZ	2.17	0.60
1:A:258:GLN:HG2	1:A:283:LEU:HD21	1.83	0.60
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.84	0.60
2:B:253:THR:HA	2:B:292:VAL:HA	1.84	0.60
2:B:306:ASN:O	2:B:308:GLU:N	2.34	0.60
2:B:395:LYS:HG2	2:B:399:GLU:OE1	2.01	0.60
1:A:108:VAL:HG23	1:A:108:VAL:O	2.02	0.60
1:A:388:LYS:NZ	4:A:1155:HOH:O	2.28	0.60
2:B:27:THR:HG22	2:B:29:GLU:HB3	1.82	0.60
2:B:376:THR:O	2:B:380:ILE:HG13	2.01	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:55:PRO:HB2	1:A:143:ARG:NH2	2.17	0.60
1:A:57:ASN:OD1	1:A:131:THR:HB	2.01	0.60
1:A:503:LEU:CG	1:A:507:GLN:HE22	2.13	0.60
1:A:226:PRO:HG3	1:A:235:HIS:HE1	1.64	0.60
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.67	0.60
2:B:61:PHE:HB3	4:B:1121:HOH:O	2.02	0.59
1:A:3:SER:HB2	1:A:4:PRO:HD2	1.83	0.59
1:A:183:TYR:HE2	1:A:230:MET:SD	2.23	0.59
2:B:224:GLU:HG3	4:B:1151:HOH:O	2.01	0.59
1:A:10:VAL:CG1	1:A:11:LYS:N	2.65	0.59
1:A:134:SER:HB2	1:A:139:THR:OG1	2.02	0.59
1:A:195:ILE:HD11	1:A:199:ARG:CZ	2.32	0.59
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.38	0.59
1:A:332:GLN:OE1	1:A:338:THR:HG23	2.02	0.59
2:B:105:SER:O	2:B:190:GLY:HA2	2.02	0.59
1:A:125:ARG:O	1:A:128:THR:OG1	2.20	0.59
1:A:131:THR:OG1	1:A:143:ARG:HG3	2.01	0.59
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.38	0.59
1:A:503:LEU:CG	1:A:507:GLN:NE2	2.64	0.59
1:A:21:VAL:HG21	1:A:59:PRO:HD3	1.83	0.59
2:B:84:THR:O	2:B:86:ASP:N	2.36	0.59
2:B:60:VAL:CG1	2:B:130:PHE:HB2	2.33	0.58
2:B:308:GLU:C	2:B:310:LEU:H	2.06	0.58
2:B:374:LYS:O	2:B:378:GLU:HG3	2.03	0.58
1:A:17:ASP:O	1:A:83:ARG:HD3	2.03	0.58
1:A:402:TRP:HE3	1:A:402:TRP:O	1.86	0.58
2:B:195:ILE:HD13	2:B:199:ARG:HH21	1.69	0.58
1:A:501:TYR:CD1	1:A:505:ILE:HD11	2.38	0.58
2:B:277:ARG:H	2:B:277:ARG:CD	1.96	0.58
1:A:356:ARG:HG3	1:A:356:ARG:HH11	1.68	0.58
2:B:4:PRO:HG3	2:B:117:SER:HB2	1.85	0.58
2:B:27:THR:HG22	2:B:30:LYS:H	1.68	0.58
1:A:173:LYS:O	1:A:176:PRO:HD3	2.04	0.58
1:A:84:THR:HG22	1:A:124:PHE:HZ	1.69	0.58
1:A:182:GLN:HB3	1:A:187:LEU:HD12	1.85	0.57
1:A:253:THR:O	1:A:256:ASP:N	2.35	0.57
2:B:274:ILE:HG23	2:B:306:ASN:CG	2.23	0.57
1:A:329:ILE:HD12	1:A:391:LEU:HD22	1.87	0.57
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.86	0.57
1:A:382:ILE:HG23	2:B:136:ASN:HD21	1.67	0.57
2:B:63:ILE:HD13	2:B:74:LEU:HD22	1.85	0.57



	louo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:60:VAL:HG13	2:B:130:PHE:HB2	1.87	0.57
1:A:19:PRO:O	1:A:56:TYR:CB	2.53	0.57
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.70	0.57
2:B:342:TYR:CD1	2:B:342:TYR:C	2.78	0.57
1:A:100:LEU:HD21	3:A:701:ADB:CL2	2.41	0.57
1:A:81:ASN:O	1:A:83:ARG:N	2.38	0.57
1:A:100:LEU:HD22	3:A:701:ADB:C8	2.35	0.56
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.40	0.56
1:A:130:PHE:CE1	1:A:144:TYR:HB2	2.39	0.56
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.26	0.56
1:A:3:SER:HB3	1:A:212:TRP:C	2.26	0.56
1:A:32:LYS:O	1:A:36:GLU:HG3	2.05	0.56
1:A:116:PHE:O	1:A:148:VAL:HG11	2.03	0.56
1:A:356:ARG:NH1	1:A:358:ARG:O	2.38	0.56
1:A:506:ILE:CG2	1:A:507:GLN:N	2.68	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.88	0.56
2:B:376:THR:HB	2:B:410:TRP:CH2	2.39	0.56
1:A:121:ASP:O	1:A:122:GLU:C	2.43	0.56
2:B:222:GLN:HG2	2:B:223:LYS:N	2.21	0.56
1:A:22:LYS:CG	1:A:24:TRP:CZ2	2.83	0.56
2:B:5:ILE:CG2	2:B:6:GLU:H	2.11	0.56
2:B:13:LYS:O	2:B:16:MET:HB2	2.04	0.56
1:A:288:ALA:CB	1:A:291:GLU:CB	2.72	0.56
2:B:231:GLY:O	2:B:233:GLU:HG3	2.06	0.56
2:B:306:ASN:C	2:B:308:GLU:H	2.09	0.56
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.38	0.56
1:A:497:THR:HG22	1:A:498:ASP:H	1.66	0.56
2:B:79:GLU:OE2	2:B:83:ARG:NH1	2.37	0.56
1:A:229:TRP:CE2	1:A:230:MET:HG2	2.40	0.56
1:A:362:THR:HG22	1:A:363:ASN:N	2.19	0.56
1:A:433:PRO:CG	2:B:255:ASN:HD22	2.18	0.56
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.06	0.56
1:A:235:HIS:HB2	1:A:238:LYS:O	2.06	0.56
2:B:168:LEU:CD1	2:B:180:ILE:HG21	2.35	0.55
2:B:222:GLN:HG2	2:B:223:LYS:H	1.70	0.55
2:B:345:PRO:HB2	2:B:346:PHE:CE1	2.42	0.55
1:A:186:ASP:HB3	1:A:188:TYR:CE1	2.40	0.55
2:B:98:ALA:O	2:B:101:LYS:HE2	2.07	0.55
2:B:395:LYS:CG	2:B:399:GLU:OE1	2.55	0.55
1:A:356:ARG:HG3	1:A:356:ARG:NH1	2.21	0.55
2:B:61:PHE:HE1	2:B:76:ASP:HB2	1.70	0.55



	i agem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:277:ARG:CD	1:A:334:GLN:HB3	2.36	0.55
1:A:433:PRO:HD3	2:B:255:ASN:ND2	2.22	0.55
2:B:206:ARG:HB3	2:B:206:ARG:CZ	2.37	0.55
2:B:245:VAL:HG12	2:B:246:LEU:O	2.06	0.55
2:B:419:THR:O	2:B:420:PRO:C	2.42	0.55
2:B:10:VAL:HG22	2:B:88:TRP:CH2	2.41	0.55
2:B:146:TYR:CD1	2:B:150:PRO:HB3	2.41	0.55
1:A:434:ILE:N	1:A:494:ASN:HD21	2.04	0.55
1:A:19:PRO:O	1:A:57:ASN:N	2.40	0.55
2:B:246:LEU:HD23	2:B:246:LEU:N	2.22	0.55
2:B:301:LEU:O	2:B:305:GLU:HB3	2.07	0.55
2:B:308:GLU:C	2:B:310:LEU:N	2.59	0.55
1:A:369:THR:CG2	1:A:398:TRP:HH2	2.19	0.55
2:B:195:ILE:HD11	2:B:233:GLU:OE1	2.06	0.55
1:A:29:GLU:O	1:A:32:LYS:HE2	2.07	0.54
2:B:328:GLU:HB3	4:B:1149:HOH:O	2.06	0.54
1:A:175:ASN:HB3	1:A:178:ILE:CD1	2.37	0.54
1:A:242:GLN:O	1:A:243:PRO:C	2.46	0.54
2:B:78:ARG:HD3	2:B:411:ILE:O	2.07	0.54
2:B:330:GLN:HG2	2:B:338:THR:OG1	2.08	0.54
1:A:18:GLY:HA3	1:A:56:TYR:CD2	2.42	0.54
2:B:2:ILE:HG23	2:B:2:ILE:O	2.06	0.54
1:A:55:PRO:HB2	1:A:143:ARG:CZ	2.36	0.54
1:A:82:LYS:O	1:A:82:LYS:HG2	2.08	0.54
1:A:182:GLN:HA	1:A:187:LEU:HA	1.89	0.54
1:A:341:ILE:HG21	1:A:383:TRP:CH2	2.42	0.54
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.43	0.54
2:B:206:ARG:NH1	2:B:216:THR:OG1	2.40	0.54
2:B:296:THR:H	2:B:299:ALA:HB3	1.73	0.54
1:A:287:LYS:HG2	1:A:288:ALA:N	2.21	0.54
2:B:73:LYS:HE2	2:B:75:VAL:HG22	1.90	0.54
2:B:362:THR:CG2	2:B:367:GLN:HG3	2.38	0.54
1:A:215:THR:HG22	1:A:216:THR:N	2.23	0.54
1:A:399:GLU:HA	1:A:402:TRP:CD1	2.43	0.54
1:A:429:LEU:HD11	1:A:506:ILE:CG2	2.38	0.54
2:B:125:ARG:O	2:B:127:TYR:N	2.40	0.54
1:A:139:THR:HB	1:A:140:PRO:CD	2.37	0.53
1:A:315:HIS:CE1	1:A:347:LYS:CD	2.90	0.53
1:A:90:VAL:CG1	1:A:91:GLN:HG3	2.33	0.53
2:B:136:ASN:O	2:B:137:ASN:HB2	2.08	0.53
2:B:156:SER:H	2:B:157:PRO:HD2	1.72	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:206:ARG:HB3	2:B:206:ARG:HH11	1.70	0.53
1:A:112:GLY:HA2	1:A:185:ASP:OD1	2.09	0.53
1:A:257:ILE:CG2	1:A:283:LEU:HD13	2.38	0.53
2:B:276:VAL:O	2:B:279:LEU:N	2.40	0.53
2:B:330:GLN:H	2:B:330:GLN:NE2	2.06	0.53
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.53
2:B:300:GLU:OE1	2:B:300:GLU:HA	2.08	0.53
1:A:335:GLY:HA2	1:A:367:GLN:NE2	2.23	0.53
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.39	0.53
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.43	0.53
1:A:304:ALA:O	1:A:307:ARG:N	2.33	0.53
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.39	0.53
2:B:340:GLN:N	2:B:340:GLN:CD	2.62	0.53
1:A:276:VAL:HG12	1:A:276:VAL:O	2.07	0.53
1:A:362:THR:CG2	1:A:363:ASN:N	2.71	0.53
1:A:28:GLU:HB3	1:A:135:ILE:CD1	2.37	0.53
1:A:54:ASN:N	1:A:55:PRO:HD3	2.24	0.53
1:A:117:SER:CB	1:A:214:LEU:HD23	2.39	0.53
1:A:54:ASN:O	1:A:55:PRO:C	2.46	0.52
1:A:50:ILE:CG1	1:A:51:GLY:N	2.71	0.52
1:A:507:GLN:C	1:A:509:GLN:H	2.11	0.52
1:A:81:ASN:C	1:A:83:ARG:N	2.63	0.52
1:A:297:GLU:HB2	1:A:298:GLU:OE2	2.10	0.52
1:A:194:GLU:O	1:A:196:GLY:N	2.42	0.52
1:A:393:ILE:HG23	1:A:414:TRP:CZ3	2.45	0.52
2:B:11:LYS:HG2	2:B:12:LEU:O	2.10	0.52
2:B:84:THR:O	2:B:87:PHE:N	2.43	0.52
2:B:91:GLN:O	2:B:92:LEU:HD23	2.10	0.52
2:B:120:LEU:O	2:B:121:ASP:C	2.48	0.52
2:B:220:LYS:HD2	2:B:231:GLY:N	2.25	0.52
1:A:27:THR:O	1:A:28:GLU:C	2.48	0.52
2:B:191:SER:OG	2:B:198:HIS:ND1	2.24	0.52
1:A:50:ILE:HG13	1:A:51:GLY:H	1.75	0.52
1:A:191:SER:OG	1:A:198:HIS:ND1	2.38	0.52
2:B:406:TRP:NE1	2:B:408:ALA:HB3	2.25	0.52
1:A:340:GLN:CB	1:A:351:THR:HG22	2.39	0.52
1:A:19:PRO:O	1:A:56:TYR:HB3	2.10	0.52
1:A:240:THR:HG23	1:A:241:VAL:N	2.24	0.52
1:A:494:ASN:HD22	2:B:289:LEU:HD12	1.74	0.52
2:B:314:VAL:HG13	2:B:317:VAL:HG21	1.92	0.52
1:A:21:VAL:CG2	1:A:59:PRO:HD3	2.40	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:460:ASN:ND2	1:A:461:LYS:H	2.08	0.51
2:B:57:ASN:HA	2:B:129:ALA:O	2.11	0.51
2:B:168:LEU:HD13	2:B:180:ILE:HG21	1.92	0.51
2:B:194:GLU:O	2:B:195:ILE:C	2.49	0.51
1:A:88:TRP:HA	1:A:88:TRP:CE3	2.45	0.51
1:A:356:ARG:HD2	1:A:358:ARG:HG3	1.91	0.51
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.92	0.51
2:B:184:MET:HE3	4:B:1037:HOH:O	2.08	0.51
1:A:117:SER:HB2	1:A:214:LEU:HD23	1.91	0.51
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.45	0.51
1:A:188:TYR:CD2	3:A:701:ADB:H5	2.45	0.51
1:A:509:GLN:N	1:A:510:PRO:CD	2.73	0.51
1:A:407:GLN:OE1	2:B:394:GLN:N	2.44	0.51
1:A:420:PRO:HA	1:A:421:PRO:O	2.09	0.51
1:A:112:GLY:C	1:A:114:ALA:H	2.14	0.51
2:B:221:HIS:N	2:B:221:HIS:CD2	2.79	0.51
2:B:225:PRO:C	2:B:227:PHE:H	2.14	0.51
1:A:277:ARG:HD2	1:A:334:GLN:HB2	1.90	0.51
1:A:402:TRP:CE3	1:A:402:TRP:C	2.84	0.51
2:B:242:GLN:HB2	2:B:243:PRO:HD2	1.93	0.51
2:B:394:GLN:O	2:B:395:LYS:C	2.48	0.51
1:A:287:LYS:HE2	1:A:291:GLU:OE1	2.11	0.51
1:A:115:TYR:CE2	1:A:151:GLN:HA	2.45	0.51
1:A:229:TRP:O	1:A:232:TYR:N	2.40	0.51
2:B:249:LYS:HD2	2:B:252:TRP:HZ3	1.73	0.51
2:B:296:THR:H	2:B:299:ALA:CB	2.24	0.51
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.92	0.51
1:A:503:LEU:HD22	1:A:535:TRP:CB	2.31	0.51
2:B:330:GLN:HE21	2:B:338:THR:C	2.14	0.51
1:A:102:LYS:O	1:A:103:LYS:HD3	2.11	0.50
1:A:424:LYS:HD3	1:A:425:LEU:H	1.73	0.50
1:A:77:PHE:CE1	1:A:150:PRO:HB3	2.47	0.50
1:A:288:ALA:HB2	1:A:291:GLU:HB2	1.89	0.50
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.77	0.50
2:B:85:GLN:HA	2:B:88:TRP:HB2	1.93	0.50
2:B:306:ASN:C	2:B:308:GLU:N	2.64	0.50
2:B:363:ASN:HD22	2:B:364:ASP:N	2.08	0.50
1:A:3:SER:CB	1:A:4:PRO:HD2	2.41	0.50
1:A:168:LEU:O	1:A:169:GLU:C	2.48	0.50
2:B:65:LYS:CA	2:B:72:ARG:HG3	2.31	0.50
1:A:58:THR:HG22	1:A:76:ASP:O	2.12	0.50



	louis page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:372:VAL:HG11	1:A:411:ILE:HG13	1.94	0.50
1:A:417:VAL:HG12	1:A:419:THR:CG2	2.40	0.50
1:A:246:LEU:HD22	1:A:260:LEU:CD1	2.42	0.50
1:A:501:TYR:C	1:A:505:ILE:HD12	2.32	0.50
2:B:171:PHE:CB	4:B:1153:HOH:O	2.60	0.50
2:B:193:LEU:HD12	2:B:198:HIS:N	2.27	0.50
1:A:507:GLN:C	1:A:509:GLN:N	2.65	0.50
2:B:85:GLN:CG	2:B:154:LYS:HB2	2.41	0.50
2:B:276:VAL:O	2:B:280:SER:N	2.33	0.50
2:B:306:ASN:HA	2:B:309:ILE:HG22	1.93	0.50
1:A:17:ASP:O	1:A:83:ARG:CD	2.59	0.50
1:A:277:ARG:HH22	1:A:514:GLU:HG3	1.76	0.50
2:B:195:ILE:HD13	2:B:199:ARG:NH2	2.27	0.50
2:B:232:TYR:CE1	2:B:234:LEU:HD21	2.46	0.49
2:B:340:GLN:OE1	2:B:340:GLN:N	2.45	0.49
1:A:94:ILE:HD13	1:A:230:MET:HE2	1.94	0.49
1:A:162:SER:HB2	2:B:52:PRO:CG	2.42	0.49
2:B:326:ILE:CG2	2:B:342:TYR:CE1	2.94	0.49
2:B:411:ILE:HG22	2:B:412:PRO:O	2.12	0.49
1:A:186:ASP:HB3	1:A:188:TYR:HE1	1.76	0.49
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.47	0.49
2:B:362:THR:HG23	2:B:366:LYS:HZ2	1.77	0.49
1:A:500:GLN:O	1:A:501:TYR:C	2.50	0.49
2:B:27:THR:O	2:B:31:ILE:HD12	2.13	0.49
2:B:345:PRO:C	2:B:346:PHE:CD1	2.86	0.49
1:A:96:HIS:CE1	1:A:350:LYS:HE2	2.48	0.49
1:A:173:LYS:C	1:A:175:ASN:H	2.16	0.49
1:A:203:GLU:O	1:A:206:ARG:HB3	2.13	0.49
2:B:22:LYS:N	2:B:22:LYS:HD2	2.28	0.49
2:B:85:GLN:C	2:B:85:GLN:OE1	2.51	0.49
2:B:221:HIS:NE2	2:B:230:MET:CE	2.75	0.49
1:A:116:PHE:HE2	1:A:146:TYR:HE1	1.61	0.49
2:B:23:GLN:OE1	2:B:60:VAL:HG22	2.12	0.49
1:A:20:LYS:HA	1:A:57:ASN:H	1.77	0.49
1:A:30:LYS:O	1:A:33:ALA:HB3	2.13	0.49
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.95	0.49
1:A:215:THR:HG22	1:A:216:THR:H	1.77	0.49
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.12	0.49
2:B:393:ILE:HG23	2:B:393:ILE:O	2.13	0.49
1:A:8:VAL:O	1:A:121:ASP:HB2	2.13	0.48
1:A:57:ASN:ND2	1:A:58:THR:H	2.10	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:104:LYS:HE3	1:A:192:ASP:OD1	2.13	0.48
1:A:343:GLN:HG3	1:A:349:LEU:HD22	1.95	0.48
1:A:376:THR:HG23	1:A:386:THR:CG2	2.41	0.48
1:A:379:SER:HA	1:A:383:TRP:CE3	2.48	0.48
2:B:135:ILE:O	2:B:138:GLU:HG3	2.12	0.48
2:B:373:GLN:NE2	2:B:406:TRP:HA	2.26	0.48
1:A:182:GLN:H	1:A:182:GLN:NE2	2.10	0.48
1:A:499:SER:OG	1:A:502:ALA:HB3	2.13	0.48
2:B:42:GLU:OE1	2:B:49:LYS:HE3	2.13	0.48
2:B:88:TRP:CB	4:B:1089:HOH:O	2.61	0.48
1:A:5:ILE:CD1	1:A:167:ILE:HD11	2.44	0.48
2:B:314:VAL:CG2	2:B:315:HIS:N	2.77	0.48
1:A:22:LYS:HG2	1:A:24:TRP:HZ2	1.70	0.48
2:B:12:LEU:HD12	2:B:12:LEU:H	1.77	0.48
2:B:246:LEU:HD12	2:B:303:LEU:HD11	1.96	0.48
2:B:325:LEU:HD12	2:B:385:LYS:HG3	1.95	0.48
1:A:34:LEU:HB2	1:A:132:ILE:HD12	1.96	0.48
1:A:229:TRP:O	1:A:232:TYR:HB2	2.13	0.48
1:A:286:THR:O	1:A:286:THR:CG2	2.59	0.48
1:A:9:PRO:0	1:A:9:PRO:HG2	2.14	0.48
1:A:135:ILE:O	1:A:135:ILE:HG13	2.12	0.48
1:A:441:TYR:CD2	1:A:542:ILE:HD12	2.48	0.48
1:A:540:LYS:O	1:A:541:GLY:O	2.30	0.48
2:B:246:LEU:HD12	2:B:303:LEU:CD1	2.44	0.48
1:A:285:GLY:HA3	1:A:287:LYS:NZ	2.28	0.48
2:B:195:ILE:CD1	2:B:199:ARG:NE	2.77	0.48
2:B:326:ILE:HG21	2:B:342:TYR:CE1	2.47	0.48
2:B:422:LEU:HD12	2:B:425:LEU:CD1	2.40	0.48
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.77	0.48
2:B:60:VAL:HG11	2:B:130:PHE:HD2	1.75	0.48
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.48	0.48
1:A:13:LYS:HD2	1:A:16:MET:CE	2.43	0.48
2:B:246:LEU:HD21	2:B:310:LEU:CD1	2.44	0.48
1:A:354:TYR:HA	4:A:1141:HOH:O	2.13	0.48
1:A:58:THR:HG22	1:A:59:PRO:CD	2.40	0.47
2:B:30:LYS:HD3	2:B:71:TRP:CH2	2.49	0.47
2:B:195:ILE:CG2	2:B:196:GLY:N	2.77	0.47
1:A:53:GLU:N	1:A:55:PRO:HD3	2.29	0.47
2:B:27:THR:HG23	4:B:1003:HOH:O	2.12	0.47
2:B:76:ASP:OD2	2:B:78:ARG:NH2	2.38	0.47
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.65	0.47



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:240:THR:HG23	1:A:241:VAL:O	2.14	0.47
1:A:326:ILE:CD1	1:A:343:GLN:HA	2.45	0.47
1:A:522:ILE:O	1:A:525:LEU:HB2	2.14	0.47
1:A:20:LYS:HG2	1:A:56:TYR:HA	1.96	0.47
1:A:223:LYS:H	1:A:223:LYS:CD	2.27	0.47
2:B:161:GLN:O	2:B:162:SER:C	2.53	0.47
2:B:198:HIS:O	2:B:199:ARG:C	2.52	0.47
1:A:56:TYR:H	1:A:56:TYR:HD1	1.58	0.47
1:A:64:LYS:CE	1:A:68:SER:CB	2.91	0.47
2:B:344:GLU:O	2:B:345:PRO:C	2.52	0.47
2:B:23:GLN:HG3	2:B:23:GLN:O	2.15	0.47
2:B:298:GLU:O	2:B:301:LEU:CB	2.62	0.47
1:A:182:GLN:H	1:A:182:GLN:CD	2.18	0.47
1:A:369:THR:HG23	1:A:398:TRP:HH2	1.79	0.47
2:B:232:TYR:HE1	2:B:234:LEU:HD21	1.80	0.47
1:A:258:GLN:HG2	1:A:283:LEU:CD2	2.44	0.47
1:A:301:LEU:HD12	1:A:301:LEU:C	2.35	0.47
2:B:346:PHE:CD1	2:B:346:PHE:N	2.82	0.47
2:B:419:THR:O	2:B:421:PRO:N	2.48	0.47
1:A:96:HIS:CE1	1:A:269:GLN:HE21	2.33	0.46
1:A:254:VAL:HA	1:A:257:ILE:HG22	1.97	0.46
1:A:278:GLN:HG2	1:A:302:GLU:OE2	2.15	0.46
1:A:410:TRP:HB2	2:B:365:VAL:HG21	1.97	0.46
1:A:344:GLU:HA	1:A:345:PRO:HD3	1.66	0.46
2:B:305:GLU:O	2:B:308:GLU:HB3	2.16	0.46
1:A:279:LEU:HD23	1:A:299:ALA:CB	2.34	0.46
2:B:85:GLN:HB2	2:B:154:LYS:HB2	1.95	0.46
2:B:206:ARG:NH1	2:B:216:THR:HG1	2.12	0.46
2:B:375:ILE:HB	2:B:389:PHE:HZ	1.80	0.46
1:A:173:LYS:O	1:A:175:ASN:N	2.48	0.46
2:B:11:LYS:NZ	2:B:14:PRO:HG3	2.31	0.46
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.95	0.46
1:A:24:TRP:N	1:A:25:PRO:CD	2.79	0.46
2:B:2:ILE:O	2:B:3:SER:C	2.54	0.46
1:A:53:GLU:C	1:A:55:PRO:CD	2.80	0.46
1:A:308:GLU:O	1:A:312:GLU:OE1	2.33	0.46
1:A:402:TRP:HE3	1:A:402:TRP:C	2.19	0.46
3:A:701:ADB:H16	3:A:701:ADB:N1	2.31	0.46
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.97	0.46
2:B:277:ARG:HA	2:B:280:SER:OG	2.16	0.46
2:B:411:ILE:O	2:B:412:PRO:O	2.34	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:329:ILE:HA	1:A:338:THR:O	2.16	0.46
1:A:540:LYS:HG3	1:A:541:GLY:N	2.31	0.46
2:B:246:LEU:HD21	2:B:310:LEU:HD13	1.98	0.46
1:A:3:SER:HB3	1:A:212:TRP:O	2.15	0.46
1:A:170:PRO:HG2	1:A:171:PHE:H	1.80	0.46
1:A:331:LYS:HZ3	1:A:333:GLY:HA2	1.80	0.46
1:A:506:ILE:HD11	1:A:521:ILE:HG21	1.97	0.46
2:B:169:GLU:N	2:B:170:PRO:HD2	2.30	0.46
2:B:222:GLN:CG	2:B:223:LYS:H	2.29	0.46
1:A:13:LYS:HD2	1:A:16:MET:HE1	1.96	0.46
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.98	0.46
2:B:96:HIS:HA	2:B:97:PRO:HD2	1.82	0.46
2:B:115:TYR:O	2:B:117:SER:N	2.49	0.46
1:A:244:ILE:CD1	1:A:310:LEU:HD13	2.19	0.45
1:A:288:ALA:HB1	1:A:291:GLU:H	1.81	0.45
1:A:394:GLN:O	1:A:395:LYS:C	2.53	0.45
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.80	0.45
1:A:438:GLU:OE1	1:A:463:ARG:NH2	2.49	0.45
1:A:85:GLN:HE22	2:B:53:GLU:HB2	1.81	0.45
1:A:426:TRP:O	1:A:427:TYR:HB3	2.16	0.45
1:A:429:LEU:HD11	1:A:506:ILE:HG23	1.98	0.45
1:A:497:THR:CG2	1:A:498:ASP:H	2.27	0.45
2:B:319:TYR:O	2:B:321:PRO:HD3	2.17	0.45
1:A:120:LEU:O	1:A:122:GLU:N	2.49	0.45
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.29	0.45
1:A:104:LYS:CE	1:A:192:ASP:OD1	2.64	0.45
1:A:356:ARG:HG2	1:A:367:GLN:HG3	1.98	0.45
2:B:139:THR:HG23	2:B:140:PRO:CD	2.44	0.45
1:A:53:GLU:H	1:A:55:PRO:HD3	1.80	0.45
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.99	0.45
1:A:379:SER:CB	1:A:387:PRO:HD3	2.47	0.45
1:A:398:TRP:O	1:A:400:THR:N	2.49	0.45
1:A:418:ASN:C	1:A:419:THR:HG22	2.37	0.45
1:A:504:GLY:O	1:A:505:ILE:C	2.54	0.45
1:A:18:GLY:HA2	1:A:19:PRO:HD3	1.84	0.45
2:B:319:TYR:CE2	2:B:321:PRO:HG3	2.52	0.45
1:A:118:VAL:HA	1:A:119:PRO:HD3	1.69	0.45
1:A:136:ASN:C	1:A:138:GLU:H	2.17	0.45
1:A:416:PHE:CE2	1:A:418:ASN:HB2	2.51	0.45
2:B:46:LYS:HD3	2:B:116:PHE:CE1	2.52	0.45
2:B:202:ILE:O	2:B:205:LEU:N	2.50	0.45



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:B:198:HIS:O	2:B:201:LYS:N	2.50	0.45
2:B:324:ASP:O	2:B:343:GLN:HG2	2.17	0.45
2:B:160:PHE:O	2:B:161:GLN:C	2.55	0.45
2:B:363:ASN:ND2	2:B:365:VAL:N	2.65	0.45
1:A:410:TRP:HB2	2:B:365:VAL:CG2	2.46	0.45
1:A:513:SER:O	1:A:519:ASN:ND2	2.50	0.45
1:A:529:GLU:C	1:A:530:LYS:HG3	2.37	0.45
2:B:153:TRP:O	2:B:155:GLY:N	2.48	0.45
2:B:171:PHE:HB3	4:B:1153:HOH:O	2.15	0.44
1:A:395:LYS:HE2	1:A:399:GLU:OE1	2.16	0.44
1:A:102:LYS:HG2	1:A:104:LYS:HZ3	1.83	0.44
1:A:235:HIS:HB2	1:A:238:LYS:CG	2.47	0.44
2:B:205:LEU:O	2:B:206:ARG:C	2.54	0.44
2:B:267:ALA:O	2:B:269:GLN:N	2.51	0.44
2:B:274:ILE:HG22	2:B:275:LYS:N	2.32	0.44
2:B:345:PRO:C	2:B:346:PHE:HD1	2.20	0.44
1:A:126:LYS:HE2	1:A:126:LYS:HB3	1.69	0.44
1:A:253:THR:O	1:A:254:VAL:C	2.56	0.44
1:A:369:THR:HG23	1:A:398:TRP:CH2	2.53	0.44
2:B:209:LEU:HD22	2:B:214:LEU:HD12	1.99	0.44
2:B:257:ILE:HD11	2:B:279:LEU:O	2.18	0.44
2:B:339:TYR:CG	2:B:375:ILE:HD13	2.52	0.44
1:A:60:VAL:HG22	1:A:130:PHE:HB2	2.00	0.44
1:A:181:TYR:CD2	1:A:181:TYR:C	2.90	0.44
1:A:412:PRO:O	1:A:414:TRP:HD1	2.01	0.44
2:B:163:SER:O	2:B:167:ILE:HG13	2.17	0.44
2:B:366:LYS:O	2:B:370:GLU:HG3	2.18	0.44
1:A:253:THR:O	1:A:256:ASP:HB2	2.18	0.44
1:A:499:SER:OG	1:A:502:ALA:CB	2.66	0.44
1:A:37:ILE:O	1:A:41:MET:HB2	2.18	0.44
1:A:411:ILE:HG13	1:A:412:PRO:HD2	2.00	0.44
1:A:435:VAL:HA	2:B:290:THR:OG1	2.18	0.44
1:A:504:GLY:O	1:A:507:GLN:N	2.50	0.44
2:B:139:THR:HG22	2:B:140:PRO:O	2.17	0.44
2:B:220:LYS:HD2	2:B:230:MET:C	2.38	0.44
2:B:234:LEU:HD11	2:B:377:THR:HG21	1.99	0.44
2:B:275:LYS:HB2	2:B:302:GLU:OE1	2.18	0.44
1:A:80:LEU:O	1:A:84:THR:HG23	2.17	0.44
1:A:231:GLY:O	1:A:242:GLN:HG2	2.18	0.44
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.87	0.44
1:A:104:LYS:N	1:A:104:LYS:CE	2.75	0.44



	h i c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.44
1:A:320:ASP:OD2	1:A:322:SER:OG	2.36	0.44
1:A:330:GLN:HE21	1:A:330:GLN:HB3	1.61	0.44
1:A:354:TYR:CZ	1:A:370:GLU:HB3	2.53	0.44
2:B:40:GLU:O	2:B:41:MET:C	2.54	0.44
2:B:104:LYS:O	2:B:105:SER:OG	2.34	0.44
2:B:109:LEU:HA	2:B:218:ASP:OD2	2.18	0.44
2:B:259:LYS:O	2:B:262:GLY:N	2.50	0.44
1:A:51:GLY:O	1:A:53:GLU:N	2.51	0.43
1:A:235:HIS:HB2	1:A:238:LYS:HG2	2.00	0.43
1:A:288:ALA:HB3	1:A:291:GLU:HB3	1.95	0.43
1:A:397:THR:O	1:A:398:TRP:C	2.56	0.43
2:B:33:ALA:O	2:B:37:ILE:HG13	2.18	0.43
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.80	0.43
1:A:30:LYS:O	1:A:31:ILE:C	2.56	0.43
1:A:241:VAL:HG12	1:A:242:GLN:N	2.33	0.43
2:B:27:THR:HG21	2:B:29:GLU:HB3	1.99	0.43
2:B:255:ASN:O	2:B:258:GLN:N	2.50	0.43
2:B:395:LYS:HE2	2:B:399:GLU:OE2	2.18	0.43
2:B:411:ILE:C	2:B:412:PRO:O	2.56	0.43
1:A:57:ASN:ND2	1:A:58:THR:N	2.66	0.43
1:A:390:LYS:HB3	1:A:417:VAL:HG21	2.00	0.43
2:B:30:LYS:HD2	2:B:62:ALA:HB3	2.01	0.43
2:B:375:ILE:HD12	2:B:389:PHE:HE2	1.82	0.43
1:A:328:GLU:HG3	1:A:390:LYS:CB	2.34	0.43
1:A:342:TYR:HA	1:A:349:LEU:HB2	2.01	0.43
2:B:13:LYS:O	2:B:16:MET:CB	2.64	0.43
2:B:27:THR:HB	2:B:30:LYS:CG	2.49	0.43
2:B:46:LYS:HZ3	2:B:116:PHE:HD1	1.66	0.43
2:B:85:GLN:CB	2:B:154:LYS:HB2	2.49	0.43
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.99	0.43
2:B:195:ILE:O	2:B:198:HIS:HB3	2.19	0.43
2:B:266:TRP:CD1	2:B:422:LEU:HD23	2.53	0.43
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.79	0.43
1:A:331:LYS:HZ1	1:A:333:GLY:HA2	1.81	0.43
2:B:342:TYR:C	2:B:342:TYR:HD1	2.21	0.43
1:A:229:TRP:NE1	1:A:230:MET:HG2	2.33	0.43
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.30	0.43
2:B:303:LEU:HD22	4:B:1143:HOH:O	2.19	0.43
2:B:308:GLU:O	2:B:310:LEU:N	2.51	0.43
1:A:531:VAL:HG12	1:A:532:TYR:N	2.33	0.43



	A h C	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:195:ILE:HG12	2:B:199:ARG:HG3	2.01	0.43
2:B:366:LYS:HZ2	2:B:366:LYS:HB3	1.84	0.43
2:B:203:GLU:HA	2:B:206:ARG:HB2	2.01	0.43
2:B:257:ILE:HG23	2:B:258:GLN:N	2.33	0.43
2:B:278:GLN:CA	2:B:281:LYS:HE3	2.22	0.43
1:A:30:LYS:HA	1:A:33:ALA:CB	2.49	0.43
1:A:94:ILE:CD1	1:A:230:MET:HE2	2.49	0.43
1:A:328:GLU:CG	1:A:390:LYS:HB2	2.36	0.43
2:B:283:LEU:C	2:B:285:GLY:N	2.72	0.43
2:B:283:LEU:O	2:B:285:GLY:N	2.51	0.43
1:A:128:THR:HB	1:A:146:TYR:HB2	2.01	0.42
1:A:137:ASN:O	1:A:138:GLU:HB3	2.18	0.42
1:A:257:ILE:HG21	1:A:283:LEU:HD13	2.01	0.42
1:A:467:VAL:HA	1:A:468:PRO:HD3	1.70	0.42
1:A:491:LEU:HB3	1:A:529:GLU:HB2	2.00	0.42
2:B:329:ILE:N	4:B:1149:HOH:O	2.51	0.42
1:A:64:LYS:HD3	1:A:71:TRP:CH2	2.54	0.42
1:A:294:PRO:O	1:A:296:THR:N	2.53	0.42
1:A:424:LYS:CD	1:A:425:LEU:N	2.79	0.42
2:B:27:THR:O	2:B:28:GLU:C	2.56	0.42
2:B:30:LYS:O	2:B:31:ILE:C	2.57	0.42
2:B:168:LEU:C	2:B:170:PRO:HD2	2.40	0.42
2:B:199:ARG:O	2:B:202:ILE:HB	2.19	0.42
1:A:62:ALA:HB1	1:A:71:TRP:CD1	2.54	0.42
1:A:195:ILE:O	1:A:199:ARG:HG3	2.19	0.42
1:A:427:TYR:CD1	1:A:427:TYR:C	2.93	0.42
1:A:457:TYR:C	1:A:457:TYR:CD2	2.93	0.42
2:B:90:VAL:O	2:B:91:GLN:C	2.57	0.42
2:B:236:PRO:HA	2:B:239:TRP:CG	2.53	0.42
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.54	0.42
1:A:183:TYR:C	1:A:184:MET:CG	2.82	0.42
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.54	0.42
2:B:13:LYS:HG2	2:B:14:PRO:O	2.20	0.42
2:B:40:GLU:O	2:B:43:LYS:N	2.52	0.42
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.55	0.42
2:B:314:VAL:HG22	2:B:315:HIS:N	2.34	0.42
1:A:34:LEU:HB2	1:A:132:ILE:CD1	2.49	0.42
1:A:470:THR:O	1:A:471:ASN:CB	2.67	0.42
1:A:19:PRO:HG2	1:A:80:LEU:HB2	2.01	0.42
1:A:294:PRO:O	1:A:295:LEU:C	2.57	0.42
2:B:195:ILE:HG23	2:B:196:GLY:H	1.81	0.42



			Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:222:GLN:CG	2:B:223:LYS:N	2.83	0.42
1:A:341:ILE:O	1:A:349:LEU:HB3	2.20	0.42
2:B:362:THR:HG23	2:B:366:LYS:NZ	2.35	0.42
1:A:542:ILE:HD13	1:A:544:GLY:CA	2.50	0.42
2:B:280:SER:O	2:B:281:LYS:C	2.58	0.42
2:B:302:GLU:O	2:B:306:ASN:HB2	2.19	0.42
1:A:5:ILE:HD11	1:A:167:ILE:HD11	2.01	0.42
1:A:59:PRO:O	1:A:75:VAL:HA	2.20	0.42
1:A:97:PRO:CG	1:A:232:TYR:CE2	2.99	0.42
2:B:234:LEU:HD11	2:B:377:THR:CG2	2.50	0.42
2:B:327:ALA:HA	4:B:1124:HOH:O	2.20	0.42
1:A:34:LEU:CB	1:A:132:ILE:HD12	2.50	0.42
2:B:58:THR:N	4:B:1111:HOH:O	2.53	0.42
2:B:207:GLN:HE21	2:B:207:GLN:HB2	1.55	0.42
2:B:257:ILE:HD12	2:B:282:LEU:HD23	2.01	0.42
2:B:361:HIS:N	2:B:361:HIS:ND1	2.68	0.42
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.20	0.41
1:A:22:LYS:HB3	1:A:24:TRP:CE2	2.55	0.41
2:B:406:TRP:CE2	2:B:408:ALA:HB3	2.55	0.41
1:A:224:GLU:CB	1:A:225:PRO:CD	2.78	0.41
1:A:257:ILE:HD11	1:A:282:LEU:HB2	2.02	0.41
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.50	0.41
2:B:393:ILE:HD13	2:B:398:TRP:HB2	2.03	0.41
1:A:198:HIS:O	1:A:202:ILE:HG12	2.20	0.41
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.34	0.41
1:A:276:VAL:HG12	1:A:280:SER:OG	2.19	0.41
1:A:289:LEU:HD12	1:A:289:LEU:HA	1.78	0.41
1:A:328:GLU:O	1:A:339:TYR:HA	2.20	0.41
1:A:434:ILE:O	1:A:437:ALA:HB3	2.21	0.41
2:B:12:LEU:HD11	2:B:127:TYR:CE2	2.56	0.41
2:B:46:LYS:CD	2:B:116:PHE:CD1	3.01	0.41
2:B:356:ARG:HB2	2:B:367:GLN:HG2	2.01	0.41
1:A:73:LYS:NZ	1:A:130:PHE:CZ	2.79	0.41
2:B:130:PHE:CE1	2:B:144:TYR:HB2	2.55	0.41
2:B:254:VAL:O	2:B:257:ILE:HG23	2.20	0.41
2:B:419:THR:H	2:B:420:PRO:CD	2.33	0.41
1:A:102:LYS:HA	1:A:318:TYR:HD1	1.85	0.41
1:A:211:ARG:HG3	1:A:211:ARG:NH1	2.35	0.41
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.85	0.41
2:B:46:LYS:CD	2:B:116:PHE:HD1	2.33	0.41
1:A:11:LYS:HB2	1:A:85:GLN:OE1	2.21	0.41



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:59:PRO:HD2	1:A:76:ASP:O	2.21	0.41	
1:A:195:ILE:HG23	1:A:196:GLY:N	2.34	0.41	
1:A:369:THR:HG1	1:A:398:TRP:HH2	1.60	0.41	
1:A:398:TRP:O	1:A:399:GLU:C	2.59	0.41	
2:B:56:TYR:O	2:B:57:ASN:HB2	2.21	0.41	
2:B:84:THR:O	2:B:85:GLN:C	2.59	0.41	
2:B:88:TRP:HB2	4:B:1089:HOH:O	2.20	0.41	
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.35	0.41	
2:B:195:ILE:O	2:B:196:GLY:C	2.59	0.41	
1:A:104:LYS:CG	1:A:192:ASP:HA	2.42	0.41	
1:A:275:LYS:NZ	1:A:332:GLN:HE21	2.18	0.41	
1:A:470:THR:O	1:A:471:ASN:HB3	2.20	0.41	
1:A:542:ILE:CG1	1:A:543:GLY:N	2.79	0.41	
2:B:282:LEU:HG	2:B:293:ILE:CD1	2.35	0.41	
2:B:298:GLU:CA	2:B:301:LEU:HB2	2.51	0.41	
1:A:102:LYS:HG2	1:A:104:LYS:HZ1	1.84	0.41	
1:A:108:VAL:O	1:A:108:VAL:CG2	2.68	0.41	
1:A:215:THR:O	1:A:216:THR:HG22	2.21	0.41	
1:A:410:TRP:HE3	1:A:410:TRP:HA	1.85	0.41	
1:A:410:TRP:HA	1:A:410:TRP:CE3	2.56	0.41	
2:B:277:ARG:N	2:B:277:ARG:CD	2.70	0.41	
2:B:336:GLN:HG2	2:B:355:ALA:HB2	2.03	0.41	
1:A:3:SER:HB2	1:A:5:ILE:HG13	2.03	0.41	
1:A:178:ILE:H	1:A:178:ILE:HG13	1.62	0.41	
2:B:183:TYR:CD2	2:B:184:MET:HG3	2.55	0.41	
1:A:252:TRP:CD1	1:A:295:LEU:HD13	2.56	0.40	
1:A:281:LYS:HE3	4:A:1074:HOH:O	2.19	0.40	
1:A:298:GLU:O	1:A:299:ALA:C	2.59	0.40	
1:A:417:VAL:CG1	1:A:419:THR:CG2	3.00	0.40	
2:B:224:GLU:HA	2:B:225:PRO:HD3	1.67	0.40	
1:A:382:ILE:HG22	1:A:383:TRP:CD1	2.57	0.40	
2:B:164:MET:O	2:B:165:THR:C	2.58	0.40	
2:B:220:LYS:HD3	2:B:229:TRP:O	2.21	0.40	
1:A:131:THR:O	1:A:131:THR:CG2	2.70	0.40	
1:A:474:ASN:C	1:A:478:GLU:HG3	2.40	0.40	
2:B:156:SER:N	2:B:157:PRO:CD	2.82	0.40	
2:B:382:ILE:O	2:B:382:ILE:CG2	2.67	0.40	
1:A:132:ILE:CG2	1:A:142:ILE:O	2.69	0.40	
1:A:259:LYS:O	1:A:263:LYS:HG3	2.22	0.40	
1:A:411:ILE:HG23	1:A:411:ILE:O	2.22	0.40	
1:A:452:LEU:CD2	1:A:470:THR:HG22	2.51	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:LYS:HB2	2:B:252:TRP:CH2	2.56	0.40
1:A:235:HIS:CB	1:A:238:LYS:HG2	2.52	0.40
2:B:46:LYS:NZ	2:B:116:PHE:HD1	2.19	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	ntiles
1	А	550/560~(98%)	429 (78%)	84 (15%)	37~(7%)	1	1
2	В	425/430~(99%)	327 (77%)	68~(16%)	30~(7%)	1	1
All	All	975/990~(98%)	756 (78%)	152 (16%)	67~(7%)	1	1

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	14	PRO
1	А	28	GLU
1	А	54	ASN
1	А	122	GLU
1	А	135	ILE
1	А	137	ASN
1	А	153	TRP
1	А	195	ILE
1	А	412	PRO
1	А	538	ALA
1	А	539	HIS
1	А	541	GLY
2	В	7	THR
2	В	77	PHE
2	В	85	GLN



Mol	Chain	Res	Type
2	В	116	PHE
2	В	218	ASP
2	В	295	LEU
2	В	360	ALA
2	В	419	THR
1	А	16	MET
1	А	82	LYS
1	А	89	GLU
1	А	121	ASP
1	А	174	GLN
1	А	224	GLU
1	А	276	VAL
1	А	398	TRP
1	А	505	ILE
1	А	516	GLU
2	В	126	LYS
2	В	154	LYS
2	В	220	LYS
2	В	288	ALA
2	В	297	GLU
2	В	307	ARG
2	В	421	PRO
1	А	52	PRO
1	А	213	GLY
1	А	254	VAL
2	В	68	SER
2	В	223	LYS
2	В	232	TYR
2	В	268	SER
1	А	23	GLN
1	A	98	ALA
1	А	162	SER
1	A	237	ASP
1	А	397	THR
1	A	501	TYR
1	A	542	ILE
2	В	18	GLY
2	В	231	GLY
2	В	284	ARG
2	В	345	PRO
1	A	399	GLU
2	В	65	LYS



Mol	Chain	Res	Type
2	В	91	GLN
2	В	198	HIS
2	В	359	GLY
1	А	69	THR
2	В	420	PRO
1	А	504	GLY
2	В	313	PRO
1	А	169	GLU
2	В	3	SER
1	А	24	TRP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	494/500~(99%)	448 (91%)	46 (9%)	9 17
2	В	389/392~(99%)	350~(90%)	39 (10%)	7 14
All	All	883/892~(99%)	798~(90%)	85 (10%)	8 16

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	9	PRO
1	А	22	LYS
1	А	28	GLU
1	А	32	LYS
1	А	40	GLU
1	А	56	TYR
1	А	58	THR
1	А	67	ASP
1	А	71	TRP
1	А	91	GLN
1	А	128	THR
1	А	131	THR
1	А	135	ILE



Mol	Chain	Res	Type
1	А	161	GLN
1	А	184	MET
1	А	188	TYR
1	А	201	LYS
1	А	217	PRO
1	А	220	LYS
1	А	223	LYS
1	А	228	LEU
1	А	274	ILE
1	А	287	LYS
1	А	296	THR
1	А	300	GLU
1	А	317	VAL
1	А	330	GLN
1	А	347	LYS
1	А	349	LEU
1	А	356	ARG
1	А	358	ARG
1	А	364	ASP
1	А	369	THR
1	А	386	THR
1	А	391	LEU
1	А	394	GLN
1	А	402	TRP
1	А	407	GLN
1	А	410	TRP
1	А	419	THR
1	А	450	THR
1	А	460	ASN
1	А	465	LYS
1	A	506	ILE
1	А	511	ASP
1	А	542	ILE
2	В	1	PRO
2	В	7	THR
2	В	16	MET
2	В	22	LYS
2	В	36	GLU
2	В	67	ASP
2	В	69	THR
2	В	91	GLN
2	В	109	LEU



Mol	Chain	Res	Type
2	В	113	ASP
2	В	163	SER
2	В	165	THR
2	В	169	GLU
2	В	170	PRO
2	В	177	ASP
2	В	187	LEU
2	В	193	LEU
2	В	194	GLU
2	В	206	ARG
2	В	221	HIS
2	В	232	TYR
2	В	239	TRP
2	В	244	ILE
2	В	246	LEU
2	В	277	ARG
2	В	279	LEU
2	В	293	ILE
2	В	301	LEU
2	В	305	GLU
2	В	314	VAL
2	В	317	VAL
2	В	338	THR
2	В	363	ASN
2	В	372	VAL
2	В	374	LYS
2	В	399	GLU
2	В	403	THR
2	В	418	ASN
2	В	419	THR

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

Mol	Chain	\mathbf{Res}	Type
1	А	23	GLN
1	А	91	GLN
1	А	96	HIS
1	А	151	GLN
1	А	161	GLN
1	А	182	GLN
1	А	235	HIS
1	А	269	GLN



Mol	Chain	Res	Type
1	А	332	GLN
1	А	361	HIS
1	А	367	GLN
1	А	460	ASN
1	А	474	ASN
1	А	475	GLN
1	А	494	ASN
1	А	507	GLN
1	А	509	GLN
1	А	519	ASN
2	В	174	GLN
2	В	207	GLN
2	В	255	ASN
2	В	258	GLN
2	В	265	ASN
2	В	315	HIS
2	В	330	GLN
2	В	340	GLN
2	В	363	ASN
2	В	394	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	Mol Type Chain I	in Res Link		Bond lengths			Bond angles			
Moi Type	Chain Res			Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
3	ADB	А	701	-	27,27,27	1.81	7 (25%)	36,37,37	2.44	9 (25%)

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	ADB	А	701	-	-	0/10/10/10	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	701	ADB	C16-C11	4.23	1.46	1.39
3	А	701	ADB	C10-N4	3.70	1.41	1.33
3	А	701	ADB	C16-C15	2.80	1.43	1.38
3	А	701	ADB	C13-C12	2.56	1.43	1.38
3	А	701	ADB	C1-C2	2.33	1.45	1.40
3	А	701	ADB	C1-C6	2.27	1.45	1.40
3	А	701	ADB	C4-C5	2.14	1.43	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	701	ADB	C8-N1-C9	9.51	120.49	112.86
3	А	701	ADB	N2-C9-N1	-4.90	118.48	126.23
3	А	701	ADB	C10-N2-C9	4.37	121.14	113.75
3	А	701	ADB	C8-O7-C1	4.13	124.56	117.18
3	А	701	ADB	N3-C10-N2	-3.58	119.80	125.42
3	А	701	ADB	N3-C8-N1	-3.25	121.37	127.63
3	А	701	ADB	C1-C6-CL6	2.85	122.14	118.41
3	А	701	ADB	C1-C2-CL2	2.70	121.94	118.41
3	А	701	ADB	N4-C10-N2	2.13	120.57	117.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



1	monomer	is	involved	in	4	short	contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	701	ADB	4	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	$OWAB(Å^2)$	Q<0.9
1	А	545/560~(97%)	-0.02	19 (3%) 44 36	25, 74, 99, 105	19 (3%)
2	В	427/430 (99%)	0.13	35 (8%) 11 8	17, 61, 101, 106	14 (3%)
All	All	972/990~(98%)	0.05	54 (5%) 24 19	17, 71, 100, 106	33 (3%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	360	ALA	6.5
2	В	1	PRO	5.7
2	В	225	PRO	5.6
2	В	2	ILE	5.2
2	В	4	PRO	5.2
2	В	230	MET	5.0
2	В	231	GLY	4.9
1	А	221	HIS	4.7
1	А	141	GLY	4.4
2	В	358	ARG	4.4
2	В	304	ALA	4.3
2	В	359	GLY	4.2
2	В	222	GLN	3.7
2	В	279	LEU	3.6
2	В	245	VAL	3.6
2	В	299	ALA	3.5
2	В	226	PRO	3.5
2	В	3	SER	3.4
1	А	74	LEU	3.4
2	В	218	ASP	3.3
1	А	132	ILE	3.2
2	В	5	ILE	3.2
2	В	301	LEU	3.1
1	А	140	PRO	3.0



Mol Chain Bog Type DSP7						
Mol	Chain	Res	Type	RSRZ		
1	A	135	ILE	3.0		
2	В	223	LYS	3.0		
1	A	1	PRO	3.0		
1	А	21	VAL	2.8		
2	В	310	LEU	2.8		
2	В	296	THR	2.8		
2	В	357	MET	2.6		
1	А	78	ARG	2.6		
1	А	219	LYS	2.6		
1	А	65	LYS	2.4		
2	В	250	ASP	2.4		
1	А	253	THR	2.4		
1	А	67	ASP	2.3		
2	В	227	PHE	2.3		
2	В	409	THR	2.3		
1	А	545	ASN	2.2		
2	В	241	VAL	2.2		
2	В	232	TYR	2.1		
2	В	224	GLU	2.1		
2	В	303	LEU	2.1		
2	В	298	GLU	2.1		
1	А	252	TRP	2.1		
2	В	356	ARG	2.1		
1	А	137	ASN	2.1		
1	А	247	PRO	2.1		
2	В	294	PRO	2.1		
2	В	69	THR	2.0		
2	В	283	LEU	2.0		
1	А	66	LYS	2.0		
1	А	60	VAL	2.0		
	1			1		

_*C*,

6.2Non-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	$B-factors(A^2)$	Q<0.9
3	ADB	А	701	25/25	0.86	0.21	$41,\!56,\!65,\!73$	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.

