

Full wwPDB X-ray Structure Validation Report (i)

Mar 11, 2024 - 02:12 PM EDT

PDB ID	:	8GET
Title	:	R. hominis 2 beta-glucuronidase bound to norquetiapine-glucuronide
Authors	:	Simpson, J.B.; Redinbo, M.R.
Deposited on	:	2023-03-07
Resolution	:	2.90 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	:	2.36
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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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.



Motrie	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	757	49%	34%	• 16%						
1	В	757	^{2%} 51%	34%	• 15%						
1	С	757	3% 51%	35%	• 13%						
1	D	757	4%	37%	• 18%						

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard



residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	В	801	-	-	-	Х



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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20810 atoms, of which 140 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	Δ	630	Total	С	Ν	Ο	\mathbf{S}	0	0	0
1	A	039	5127	3262	852	992	21	0	0	0
1	В	644	Total	С	Ν	0	S	0	0	0
1	D	044	5138	3263	853	1002	20	0	0	0
1	C	650	Total	С	Ν	0	S	0	0	0
1		059	5256	3339	879	1017	21	0		0
1	П	623	Total	С	Ν	0	S	0	0	0
	025	4942	3141	828	955	18			U	

• Molecule 1 is a protein called beta-galactosidase.

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	247	ALA	THR	conflict	UNP A0A395V8I7
В	247	ALA	THR	conflict	UNP A0A395V8I7
С	247	ALA	THR	conflict	UNP A0A395V8I7
D	247	ALA	THR	conflict	UNP A0A395V8I7

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total C H O 14 3 8 3	0	0
2	В	1	Total C H O 14 3 8 3	0	0
2	В	1	Total C H O 14 3 8 3	0	0
2	В	1	Total C H O 14 3 8 3	0	0
2	С	1	Total C H O 14 3 8 3	0	0
2	С	1	Total C H O 14 3 8 3	0	0
2	D	1	Total C H O 14 3 8 3	0	0

• Molecule 3 is beta-D-glucopyranuronic acid (three-letter code: BDP) (formula: $C_6H_{10}O_7$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C H O 22 6 9 7	0	0
3	В	1	Total C H O 22 6 9 7	0	0
3	D	1	Total C H O 22 6 9 7	0	0

 $\bullet \ \ \ Molecule \ 4 \ is \ FLAVIN \ MONONUCLEOTIDE \ (three-letter \ code: \ FMN) \ (formula: \ C_{17}H_{21}N_4O_9P).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
4	А	1	Total 50	C 17	Н 19	N 4	0 9	Р 1	0	0



Continued	from	previous	page
	1	1	$I \rightarrow J$

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf			
4	Р	1	Total	С	Η	Ν	0	Р	0	0	
4	4 D	L	50	17	19	4	9	1	0	0	
4	C	1	Total	С	Η	Ν	0	Р	0	0	
4	U	L	50	17	19	4	9	1	0	0	

• Molecule 5 is 11-(4-beta-D-glucopyranuronosylpiperazin-1-yl)dibenzo[b,f][1,4]thiazepine (three-letter code: ZG5) (formula: $C_{23}H_{25}N_3O_6S$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf			
5	С	1	Total 33	C 23	N 3	0 6	S 1	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: beta-galactosidase















4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants	100.47Å 146.29Å 281.43Å	Deneiten
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\mathbf{\hat{A}})$	48.05 - 2.90	Depositor
Resolution (A)	48.05 - 2.90	EDS
% Data completeness	89.0 (48.05-2.90)	Depositor
(in resolution range)	89.0 (48.05-2.90)	EDS
R_{merge}	0.07	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.54 (at 2.91 \text{\AA})$	Xtriage
Refinement program	phenix.refine 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
D D	0.224 , 0.269	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.222 , 0.268	DCC
R_{free} test set	1999 reflections (2.42%)	wwPDB-VP
Wilson B-factor $(Å^2)$	65.6	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 53.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	20810	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 2.93% 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: GOL, FMN, BDP, ZG5 $\,$

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	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/5267	0.47	0/7165
1	В	0.28	0/5281	0.49	0/7194
1	С	0.26	0/5398	0.49	0/7345
1	D	0.25	0/5076	0.47	0/6908
All	All	0.26	0/21022	0.48	0/28612

There are no bond length outliers.

There are no bond angle outliers.

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	5127	0	4768	231	0
1	В	5138	0	4748	226	0
1	С	5256	0	4894	241	0
1	D	4942	0	4487	275	0
2	А	6	8	8	1	0
2	В	18	24	24	1	0
2	С	12	16	16	5	0
2	D	6	8	8	0	0
3	А	13	9	9	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	В	13	9	9	3	0
3	D	13	9	8	1	0
4	А	31	19	19	1	0
4	В	31	19	19	3	0
4	С	31	19	19	2	0
5	С	33	0	0	1	0
All	All	20670	140	19036	972	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 24.

All (972) 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 (Å)	overlap (Å)
1:B:168:PRO:HB3	1:B:177:VAL:HG12	1.35	1.07
1:B:371:VAL:HG23	1:B:372:VAL:HG13	1.39	1.02
1:C:166:VAL:HG22	1:C:179:VAL:HG12	1.41	1.02
1:C:367:HIS:HB2	1:C:370:ILE:HD12	1.43	0.98
1:B:175:ALA:HB3	1:B:223:VAL:HG11	1.48	0.95
1:A:367:HIS:HB2	1:A:370:ILE:HD12	1.50	0.94
1:B:72:LEU:HD23	1:B:74:LEU:HD11	1.46	0.93
1:C:562:LEU:HD13	1:C:628:SER:HB3	1.52	0.92
1:C:493:HIS:O	1:C:497:ILE:HG13	1.72	0.90
1:C:68:ASP:HB3	1:C:151:LYS:HG3	1.53	0.89
1:C:261:GLU:HG2	1:C:269:ILE:HB	1.55	0.89
1:B:183:LEU:HD21	1:B:241:LEU:HD11	1.55	0.88
1:D:183:LEU:HD21	1:D:241:LEU:HD21	1.54	0.88
1:D:395:ILE:HD12	1:D:395:ILE:H	1.37	0.88
1:D:471:ALA:HB3	1:D:544:LYS:HE3	1.56	0.88
1:C:281:SER:HB3	1:C:314:ARG:HB3	1.54	0.88
1:B:590:VAL:HG11	1:B:609:VAL:HG11	1.56	0.87
1:A:493:HIS:O	1:A:497:ILE:HG13	1.75	0.86
1:A:8:THR:HA	1:A:31:THR:HG23	1.57	0.86
1:B:91:ALA:HB2	1:B:102:VAL:HG21	1.58	0.85
1:C:198:ASP:OD1	1:C:199:ALA:N	2.09	0.85
1:A:562:LEU:HD23	1:A:579:VAL:HG22	1.57	0.84
1:B:181:VAL:HG21	1:B:239:VAL:HG11	1.60	0.84
1:D:168:PRO:HA	1:D:177:VAL:HA	1.58	0.84
1:B:358:LYS:O	1:B:362:VAL:HG23	1.78	0.83
1:C:411:ILE:HD13	1:C:427:PRO:HG3	1.59	0.83
1:A:277:LEU:HD22	1:A:334:VAL:HG21	1.60	0.83



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:168:PRO:CB	1:B:177:VAL:HG12	2.09	0.82
1:B:501:PHE:CE2	1:B:554:LEU:HD21	2.14	0.82
1:D:443:VAL:HG23	1:D:496:MET:HE2	1.61	0.82
1:D:280:VAL:HG12	1:D:511:VAL:CG1	2.09	0.82
1:C:101:ARG:HE	1:C:156:LEU:HB3	1.44	0.82
1:B:204:VAL:HG11	1:B:220:ILE:HG23	1.62	0.81
1:A:164:ILE:HD12	1:A:181:VAL:HG12	1.62	0.81
1:C:196:VAL:HG11	1:C:220:ILE:HD11	1.63	0.81
1:D:78:ASN:HA	1:D:96:GLY:HA3	1.64	0.80
1:D:154:PHE:CE1	1:D:249:ASP:HB2	2.17	0.80
1:B:362:VAL:HA	4:B:805:FMN:HM72	1.63	0.80
1:D:371:VAL:HG23	1:D:372:VAL:HG13	1.64	0.80
1:C:333:LEU:O	1:C:369:SER:HB2	1.82	0.80
1:C:464:MET:HG3	1:C:500:LEU:HD21	1.64	0.80
1:D:341:TYR:HB3	1:D:375:LEU:O	1.81	0.80
1:B:636:PHE:CZ	1:B:640:TYB:HB2	2.18	0.79
1:D:154:PHE:CZ	1:D:241:LEU:HD23	2.16	0.79
1:B:280:VAL:HG12	1:B:511:VAL:CG1	2.12	0.79
1:C:101:ARG:HH21	1:C:156:LEU:HA	1.46	0.79
1:C:59:LEU:HD11	1:C:64:LEU:HD22	1.64	0.78
1:A:281:SER:HB3	1:A:314:ARG:HB3	1.65	0.77
1:B:615:SER:HB2	1:B:630:ILE:HG12	1.65	0.77
1:B:636:PHE:HE2	1:B:641:SER:HB2	1.48	0.77
1:C:305:ILE:HG21	1:C:313:ILE:HD11	1.65	0.77
1:D:302:ILE:HD11	1:D:331:ARG:HG3	1.65	0.77
1:D:399:MET:O	1:D:403:MET:HG3	1.82	0.77
1:B:574:THR:HA	1:B:610:PRO:HA	1.65	0.77
1:A:513:ASN:O	1:A:534:GLY:HA2	1.84	0.77
1:A:592:GLY:HA2	2:A:801:GOL:H11	1.67	0.77
1:A:60:LYS:HD3	1:A:111:GLU:OE2	1.85	0.77
1:A:262:ILE:HD12	1:A:408:LEU:HD22	1.67	0.76
1:A:340:PRO:O	1:A:342:ILE:HG22	1.84	0.76
1:B:501:PHE:HE2	1:B:554:LEU:HD21	1.50	0.76
1:D:463:GLY:HA2	1:D:506:ILE:HG23	1.67	0.76
1:C:530:GLN:NE2	1:C:538:PHE:HB2	2.00	0.76
1:C:350:ARG:O	1:C:354:ILE:HD12	1.86	0.75
1:D:357:MET:O	1:D:361:VAL:HG23	1.86	0.75
1:A:170:ILE:HD11	1:A:225:LEU:HD21	1.67	0.75
1:D:470:GLU:HG2	1:D:533:LYS:HG3	1.67	0.74
1:D:623:GLU:O	1:D:623:GLU:HG3	1.86	0.74
1:B:590:VAL:HG11	1:B:609:VAL:CG1	2.17	0.74



	ie us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:379:ILE:HG23	1:A:389:LEU:HD11	1.66	0.74
1:B:362:VAL:HG13	4:B:805:FMN:C6	2.18	0.74
1:B:284:GLN:HG2	1:B:318:TYR:CE1	2.22	0.74
1:C:305:ILE:HA	1:C:514:MET:HE1	1.69	0.73
1:C:513:ASN:O	1:C:534:GLY:HA2	1.88	0.73
1:A:362:VAL:HA	4:A:803:FMN:HM72	1.70	0.73
1:A:302:ILE:HD11	1:A:331:ARG:HG3	1.70	0.73
1:C:68:ASP:CB	1:C:151:LYS:HG3	2.17	0.73
1:D:230:LYS:HE3	1:D:230:LYS:HA	1.71	0.73
1:B:636:PHE:CE2	1:B:641:SER:HB2	2.23	0.73
1:D:432:TYR:HB3	1:D:434:HIS:CD2	2.23	0.73
1:D:451:ASP:O	1:D:455:LYS:HG2	1.88	0.73
1:D:73:GLU:HB2	1:D:147:ILE:HD11	1.71	0.72
1:D:192:LEU:HD23	1:D:241:LEU:HD22	1.70	0.72
1:A:305:ILE:HA	1:A:514:MET:HE1	1.72	0.72
1:B:495:GLU:O	1:B:499:GLN:HG3	1.90	0.72
1:D:513:ASN:O	1:D:534:GLY:HA2	1.90	0.72
1:A:168:PRO:HB3	1:A:177:VAL:HG12	1.72	0.72
1:B:1:ARG:HG3	1:B:149:VAL:HG12	1.69	0.72
1:D:266:ARG:HA	1:D:504:LYS:HZ3	1.54	0.72
1:D:305:ILE:HA	1:D:514:MET:HE1	1.72	0.72
1:D:59:LEU:HD11	1:D:64:LEU:HD21	1.70	0.72
1:D:419:ILE:HD11	1:D:453:PHE:CD2	2.24	0.72
1:D:423:TYR:HA	1:D:426:ILE:CD1	2.20	0.72
1:A:415:SER:HB2	1:A:434:HIS:ND1	2.05	0.71
1:C:378:GLU:HB3	1:C:414:VAL:HB	1.73	0.71
1:B:391:GLU:O	1:B:395:ILE:HD12	1.90	0.71
1:B:404:ASP:OD2	1:B:407:ARG:HD2	1.90	0.71
1:B:207:THR:HG22	1:B:218:LEU:HD21	1.73	0.71
1:D:339:ILE:HD11	1:D:341:TYR:HB2	1.71	0.71
1:A:277:LEU:CD2	1:A:334:VAL:HG21	2.21	0.71
1:B:104:ILE:HD12	1:B:108:LEU:HD21	1.72	0.71
1:D:230:LYS:HD2	1:D:230:LYS:N	2.06	0.71
1:B:166:VAL:HG12	1:B:168:PRO:HD3	1.73	0.70
1:A:573:ASP:OD1	1:A:632:LYS:HE2	1.92	0.70
1:A:562:LEU:CD2	1:A:579:VAL:HG22	2.20	0.70
1:C:282:ARG:NH2	1:C:284:GLN:HA	2.07	0.70
1:A:101:ARG:NH2	1:A:161:GLY:O	2.21	0.70
1:C:411:ILE:CD1	1:C:427:PRO:HG3	2.20	0.70
1:C:467:TYR:CD2	1:C:496:MET:HG2	2.26	0.70
1:D:225:LEU:H	1:D:225:LEU:HD23	1.56	0.70



	, and pagern	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:273:GLU:OE1	1:D:273:GLU:N	2.24	0.70
1:A:269:ILE:HD13	1:A:274:GLU:HA	1.74	0.70
1:C:443:VAL:HG23	1:C:496:MET:CE	2.22	0.69
1:B:78:ASN:HA	1:B:96:GLY:HA3	1.74	0.69
1:B:438:TRP:CZ2	1:B:470:GLU:HG3	2.28	0.69
1:D:339:ILE:CD1	1:D:341:TYR:HB2	2.23	0.69
1:B:443:VAL:HG23	1:B:496:MET:HE2	1.73	0.69
1:C:88:LYS:HD3	1:C:107:GLU:OE1	1.91	0.69
1:B:33:PRO:HB2	1:B:292:ALA:HB1	1.74	0.69
1:D:341:TYR:CE1	1:D:379:ILE:HD11	2.27	0.69
1:D:350:ARG:HG2	1:D:354:ILE:CD1	2.22	0.69
1:D:493:HIS:HA	1:D:496:MET:HB2	1.75	0.69
1:B:262:ILE:HD12	1:B:408:LEU:HD12	1.74	0.69
1:D:360:LEU:HD12	1:D:364:ASN:HD22	1.58	0.69
1:B:168:PRO:HA	1:B:177:VAL:HA	1.75	0.69
1:B:150:ASN:OD1	1:B:151:LYS:N	2.25	0.68
1:B:280:VAL:HG12	1:B:511:VAL:HG12	1.74	0.68
1:C:302:ILE:HD13	1:C:327:LEU:HB3	1.74	0.68
1:C:302:ILE:HG23	1:C:331:ARG:HH12	1.57	0.68
1:A:379:ILE:HG21	1:A:393:HIS:HE1	1.59	0.68
1:B:220:ILE:HB	1:B:223:VAL:HG12	1.74	0.68
1:B:168:PRO:HB3	1:B:177:VAL:CG1	2.20	0.68
1:C:396:LEU:O	1:C:400:VAL:HG23	1.95	0.67
1:D:233:TYR:O	1:D:234:LEU:HD23	1.93	0.67
1:C:78:ASN:HA	1:C:96:GLY:HA3	1.75	0.67
1:B:170:ILE:HD11	1:B:257:CYS:HB3	1.75	0.67
1:D:164:ILE:HD11	1:D:239:VAL:HG13	1.77	0.67
1:D:313:ILE:HD11	1:D:333:LEU:HD13	1.77	0.67
1:A:471:ALA:HB2	1:A:489:GLN:HB2	1.77	0.67
1:C:6:PHE:CE1	1:C:57:LYS:HE2	2.30	0.67
1:D:72:LEU:HA	1:D:146:ILE:HD13	1.75	0.67
1:A:1:ARG:HB2	1:A:249:ASP:OD1	1.94	0.67
1:B:68:ASP:HB3	1:B:151:LYS:HD3	1.77	0.67
1:B:220:ILE:HB	1:B:223:VAL:CG1	2.25	0.67
1:C:576:LYS:CE	1:C:606:HIS:HB3	2.26	0.67
1:D:589:PHE:CE1	1:D:594:SER:HB2	2.29	0.67
1:B:513:ASN:O	1:B:534:GLY:HA2	1.95	0.66
1:A:316:ALA:HB1	1:A:317:HIS:ND1	2.10	0.66
1:B:333:LEU:O	1:B:369:SER:HB2	1.96	0.66
1:C:3:VAL:HG22	1:C:147:ILE:HG13	1.77	0.66
1:D:142:ARG:HD3	1:D:321:ASP:OD1	1.96	0.66



	to do pagon	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:198:ASP:CB	1:D:236:THR:H	2.08	0.66
1:A:585:GLU:OE2	1:A:597:LYS:HD2	1.95	0.66
1:A:195:THR:HG23	1:A:238:GLU:HB2	1.78	0.66
1:D:360:LEU:HD12	1:D:364:ASN:ND2	2.11	0.66
1:A:497:ILE:HD12	1:A:604:PHE:HZ	1.60	0.66
1:C:242:VAL:HG12	1:C:244:GLY:O	1.96	0.66
1:D:33:PRO:HB2	1:D:292:ALA:HB1	1.78	0.66
1:C:166:VAL:HG11	1:C:255:PHE:CD2	2.31	0.65
1:A:66:GLU:HA	1:A:70:TYR:OH	1.96	0.65
1:C:167:THR:HG22	1:C:365:TYR:HE2	1.62	0.65
1:D:225:LEU:HD12	1:D:271:ASN:CG	2.17	0.65
1:A:413:VAL:HG12	1:A:414:VAL:O	1.96	0.65
1:C:391:GLU:O	1:C:395:ILE:HG13	1.97	0.65
1:C:530:GLN:HE21	1:C:538:PHE:HB2	1.60	0.65
1:D:37:ASN:HA	1:D:40:ASP:OD1	1.96	0.65
1:D:147:ILE:HG22	1:D:149:VAL:HG13	1.78	0.65
1:C:583:LEU:HD13	1:C:584:PRO:HD2	1.79	0.65
1:A:153:HIS:ND1	1:A:156:LEU:HD12	2.12	0.65
1:B:2:GLU:OE1	1:B:4:ILE:CG1	2.45	0.65
1:D:36:TRP:HZ2	1:D:121:ASN:HD22	1.45	0.64
1:B:316:ALA:HB1	1:B:317:HIS:ND1	2.12	0.64
1:A:302:ILE:HG21	1:A:327:LEU:HD13	1.79	0.64
1:B:58:GLN:HG2	1:B:114:LEU:HD12	1.78	0.64
1:D:632:LYS:HD2	1:D:633:VAL:O	1.97	0.64
1:B:37:ASN:HA	1:B:40:ASP:OD1	1.97	0.64
1:D:259:THR:O	1:D:271:ASN:N	2.24	0.64
1:D:500:LEU:HD23	1:D:509:THR:HG22	1.78	0.64
1:A:367:HIS:HB2	1:A:370:ILE:CD1	2.25	0.64
1:B:183:LEU:HD23	1:B:186:ALA:CB	2.28	0.64
1:D:589:PHE:HE1	1:D:594:SER:HB2	1.63	0.64
1:C:97:TYR:O	1:C:319:GLN:HB3	1.97	0.64
1:A:391:GLU:O	1:A:395:ILE:HG13	1.98	0.64
1:D:284:GLN:HG2	1:D:318:TYR:CE1	2.33	0.63
1:C:339:ILE:HD13	1:C:357:MET:HE1	1.78	0.63
1:D:266:ARG:HA	1:D:504:LYS:NZ	2.12	0.63
1:B:32:LEU:HA	1:B:33:PRO:C	2.19	0.63
1:D:586:VAL:HG22	1:D:621:ALA:HB2	1.80	0.63
1:A:302:ILE:CD1	1:A:331:ARG:HG3	2.28	0.63
1:D:73:GLU:HB2	1:D:147:ILE:CD1	2.28	0.63
1:A:154:PHE:HD2	1:A:251:VAL:HG13	1.63	0.63
1:A:475:HIS:HA	1:A:487:GLU:OE1	1.98	0.63



	lo uo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:284:GLN:HG2	1:A:318:TYR:CE1	2.34	0.63
1:B:483:ASP:CG	1:B:485:THR:HG23	2.19	0.63
1:A:236:THR:HG22	1:A:254:ARG:HG2	1.80	0.62
1:C:35:SER:O	1:C:38:GLU:HG3	1.99	0.62
1:A:275:TYR:HE1	1:A:311:THR:HG21	1.64	0.62
1:D:302:ILE:CD1	1:D:331:ARG:HG3	2.29	0.62
1:C:339:ILE:HD13	1:C:357:MET:CE	2.29	0.62
1:D:419:ILE:HD11	1:D:453:PHE:HD2	1.63	0.62
1:A:83:VAL:HG22	1:A:117:ILE:HG12	1.81	0.62
1:C:626:ASP:OD1	1:C:627:GLU:N	2.33	0.62
1:B:183:LEU:HD23	1:B:186:ALA:HB2	1.80	0.62
1:B:349:GLY:O	1:B:353:THR:HG23	2.00	0.62
1:C:358:LYS:O	1:C:362:VAL:HG23	1.99	0.62
1:D:166:VAL:HG11	1:D:255:PHE:CG	2.34	0.62
1:D:333:LEU:O	1:D:369:SER:HB2	1.98	0.62
1:B:284:GLN:HG2	1:B:318:TYR:HE1	1.61	0.62
1:A:73:GLU:HB2	1:A:147:ILE:HD11	1.82	0.62
1:C:223:VAL:HG13	1:C:225:LEU:HD21	1.81	0.62
1:A:101:ARG:HH11	1:A:156:LEU:HD23	1.64	0.62
1:A:181:VAL:O	1:A:214:THR:HB	1.99	0.62
1:B:72:LEU:CD2	1:B:74:LEU:HD11	2.27	0.62
1:A:24:PRO:HG2	1:A:27:TRP:CE3	2.34	0.62
1:C:154:PHE:CD2	1:C:251:VAL:HG22	2.35	0.62
1:A:256:GLY:N	1:A:368:PRO:HG3	2.15	0.61
1:A:279:GLY:O	1:A:511:VAL:HG23	1.99	0.61
1:C:183:LEU:CD1	1:C:241:LEU:HD22	2.29	0.61
1:D:350:ARG:HG2	1:D:354:ILE:HD11	1.81	0.61
1:A:168:PRO:CB	1:A:177:VAL:HG12	2.30	0.61
1:B:280:VAL:HG21	1:B:305:ILE:HD11	1.82	0.61
1:C:167:THR:HG22	1:C:365:TYR:CE2	2.35	0.61
1:C:583:LEU:CD1	1:C:584:PRO:HD2	2.30	0.61
1:C:166:VAL:CG2	1:C:179:VAL:HG12	2.25	0.61
1:D:411:ILE:HD12	1:D:413:VAL:HG23	1.82	0.61
1:B:275:TYR:HE1	1:B:311:THR:HB	1.65	0.61
1:D:277:LEU:HD11	1:D:334:VAL:HG11	1.82	0.61
1:B:23:MET:HB2	1:B:114:LEU:HD11	1.83	0.61
1:C:313:ILE:HD12	1:C:333:LEU:HD13	1.81	0.61
1:D:192:LEU:CD1	1:D:212:GLY:HA2	2.31	0.61
1:D:300:GLU:O	1:D:304:LEU:HD12	2.01	0.61
1:B:430:ILE:HD11	1:B:453:PHE:CZ	2.35	0.61
1:D:429:VAL:HG12	1:D:461:PRO:HB2	1.82	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:202:LYS:HD2	1:A:202:LYS:N	2.14	0.61
1:A:587:GLU:HG2	1:A:589:PHE:CE2	2.36	0.61
1:D:350:ARG:O	1:D:354:ILE:HD12	2.00	0.61
1:A:101:ARG:NH1	1:A:156:LEU:HA	2.16	0.61
1:D:154:PHE:CD1	1:D:249:ASP:HB2	2.36	0.61
1:A:423:TYR:HA	1:A:426:ILE:HD12	1.81	0.60
1:A:35:SER:O	1:A:38:GLU:HG3	2.01	0.60
1:A:224:HIS:HB2	1:A:233:TYR:CD2	2.37	0.60
1:B:68:ASP:CB	1:B:151:LYS:HG2	2.31	0.60
1:C:501:PHE:CE2	1:C:554:LEU:HD21	2.36	0.60
1:B:91:ALA:HB2	1:B:102:VAL:CG2	2.30	0.60
1:C:576:LYS:HE2	1:C:606:HIS:HB3	1.82	0.60
1:C:226:TRP:CZ2	1:C:332:GLY:HA2	2.37	0.60
1:B:453:PHE:CD1	1:B:462:LEU:HD22	2.36	0.60
1:A:423:TYR:HA	1:A:426:ILE:CD1	2.32	0.60
1:B:590:VAL:CG1	1:B:609:VAL:HG11	2.28	0.60
1:C:181:VAL:O	1:C:214:THR:HB	2.02	0.60
1:C:306:CYS:SG	1:C:331:ARG:HD2	2.42	0.60
1:D:268:PHE:HE2	1:D:270:LEU:HB2	1.67	0.60
1:D:155:ASP:OD2	1:D:158:TYR:HB2	2.01	0.60
1:A:331:ARG:HB2	1:A:333:LEU:HD12	1.82	0.59
1:B:2:GLU:OE1	1:B:4:ILE:HG13	2.02	0.59
1:B:357:MET:CE	1:B:375:LEU:HD23	2.32	0.59
1:A:280:VAL:O	1:A:313:ILE:HA	2.03	0.59
1:C:207:THR:HG22	1:C:208:GLU:H	1.67	0.59
1:C:241:LEU:O	1:C:248:VAL:HG22	2.01	0.59
1:B:473:ASN:OD1	1:B:473:ASN:O	2.20	0.59
1:C:722:ILE:HD12	1:C:722:ILE:H	1.67	0.59
1:D:396:LEU:O	1:D:400:VAL:HG13	2.01	0.59
1:B:68:ASP:HB3	1:B:151:LYS:CD	2.33	0.59
1:D:298:HIS:O	1:D:302:ILE:HG22	2.02	0.59
1:C:280:VAL:O	1:C:313:ILE:HA	2.02	0.59
1:D:153:HIS:HA	1:D:249:ASP:OD2	2.03	0.59
1:D:314:ARG:HD2	1:D:336:TRP:CZ3	2.38	0.59
1:A:170:ILE:HD11	1:A:225:LEU:CD2	2.32	0.59
1:A:187:ALA:HB1	1:A:189:ASP:OD1	2.02	0.58
1:B:543:LYS:HD2	1:B:547:PHE:CE1	2.39	0.58
1:C:517:PHE:CE1	1:C:531:ASN:HB3	2.39	0.58
1:D:167:THR:HG1	1:D:365:TYR:HH	1.50	0.58
1:D:314:ARG:HD2	1:D:336:TRP:CE3	2.38	0.58
1:D:354:ILE:HD12	1:D:354:ILE:H	1.68	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:225:LEU:HD13	1:A:271:ASN:OD1	2.04	0.58
1:B:294:LEU:HD12	1:B:297:HIS:HE1	1.68	0.58
1:C:493:HIS:HE1	1:C:511:VAL:HG13	1.67	0.58
1:D:472:LEU:HD13	1:D:525:GLY:O	2.04	0.58
1:A:302:ILE:CD1	1:A:327:LEU:HB3	2.33	0.58
1:D:286:ARG:CZ	1:D:540:ARG:HD3	2.33	0.58
1:C:2:GLU:HG2	1:C:4:ILE:HD11	1.85	0.58
1:D:164:ILE:CD1	1:D:239:VAL:HG13	2.33	0.58
1:D:175:ALA:O	1:D:220:ILE:HA	2.04	0.58
1:D:35:SER:O	1:D:38:GLU:HG3	2.04	0.57
1:D:443:VAL:HG21	1:D:495:GLU:HB2	1.86	0.57
1:A:270:LEU:HD13	1:A:275:TYR:CD2	2.38	0.57
1:B:611:ASN:OD1	1:B:630:ILE:HD12	2.03	0.57
1:C:183:LEU:HD11	1:C:241:LEU:HD22	1.85	0.57
1:C:598:LEU:HB2	1:C:607:PHE:CE2	2.38	0.57
1:A:495:GLU:HA	1:A:498:LYS:HE3	1.87	0.57
1:D:51:GLY:O	1:D:120:GLU:HA	2.04	0.57
1:B:6:PHE:CE2	1:B:57:LYS:HD3	2.39	0.57
1:C:436:PHE:HB2	1:C:446:ASN:ND2	2.20	0.57
1:C:496:MET:HG3	1:C:500:LEU:HD13	1.86	0.57
1:A:611:ASN:OD1	1:A:630:ILE:HD12	2.03	0.57
1:B:400:VAL:HG21	1:B:409:THR:HG22	1.85	0.57
1:B:2:GLU:OE1	1:B:4:ILE:HG12	2.04	0.57
1:D:501:PHE:HE2	1:D:554:LEU:HD11	1.70	0.57
1:A:154:PHE:CD2	1:A:251:VAL:HG13	2.39	0.57
1:A:379:ILE:HG21	1:A:393:HIS:CE1	2.38	0.57
1:B:13:THR:HG21	1:B:16:ALA:HB2	1.87	0.57
1:B:73:GLU:OE1	1:B:101:ARG:NH1	2.38	0.57
1:D:13:THR:HG21	1:D:27:TRP:CE2	2.40	0.57
1:D:424:ILE:CG2	1:D:430:ILE:HD13	2.35	0.57
1:A:154:PHE:HE2	1:A:250:ALA:HA	1.70	0.56
1:D:574:THR:HA	1:D:610:PRO:HA	1.86	0.56
1:A:101:ARG:NH1	1:A:156:LEU:HD23	2.18	0.56
1:B:204:VAL:CG1	1:B:220:ILE:HG23	2.34	0.56
1:B:419:ILE:O	1:B:424:ILE:HD11	2.05	0.56
1:C:262:ILE:HD12	1:C:408:LEU:HD12	1.87	0.56
1:C:305:ILE:HD13	1:C:313:ILE:HD11	1.86	0.56
1:D:193:VAL:HG23	1:D:193:VAL:O	2.04	0.56
1:A:312:THR:HB	1:A:334:VAL:HG23	1.87	0.56
1:B:285:ASP:HB2	1:B:290:GLY:O	2.04	0.56
1:C:467:TYR:CE2	1:C:496:MET:HG2	2.40	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:164:ILE:HD12	1:D:251:VAL:HG13	1.86	0.56
1:D:285:ASP:HB2	1:D:290:GLY:O	2.06	0.56
1:D:549:ALA:HB2	1:D:580:TYR:CE2	2.39	0.56
1:B:399:MET:O	1:B:403:MET:HG3	2.05	0.56
1:C:101:ARG:NE	1:C:156:LEU:HB3	2.19	0.56
1:B:85:VAL:HG22	1:B:115:ILE:HD13	1.86	0.56
1:A:78:ASN:HA	1:A:96:GLY:HA3	1.87	0.56
1:C:197:LYS:HE3	1:C:238:GLU:OE1	2.06	0.56
1:D:253:THR:HG21	1:D:366:ASN:ND2	2.20	0.56
1:B:23:MET:HE2	1:B:23:MET:HA	1.87	0.56
1:B:551:LYS:HG2	1:B:559:PHE:CE2	2.41	0.56
1:D:32:LEU:HA	1:D:33:PRO:C	2.25	0.56
1:A:623:GLU:OE1	1:A:623:GLU:N	2.37	0.56
1:B:379:ILE:HG23	1:B:389:LEU:HD11	1.85	0.56
1:C:495:GLU:O	1:C:499:GLN:HG3	2.06	0.56
1:C:198:ASP:OD1	1:C:233:TYR:OH	2.21	0.56
1:D:456:GLU:C	1:D:457:PHE:HD1	2.08	0.56
1:B:92:HIS:NE2	1:B:94:ASP:OD2	2.34	0.56
1:D:36:TRP:HZ2	1:D:121:ASN:ND2	2.04	0.56
1:D:469:CYS:HB3	1:D:489:GLN:CG	2.36	0.56
1:D:503:ARG:HB2	1:D:506:ILE:HD12	1.88	0.56
1:A:225:LEU:HD22	1:A:257:CYS:O	2.05	0.55
1:C:59:LEU:HD11	1:C:64:LEU:CD2	2.33	0.55
1:C:223:VAL:HG22	1:C:225:LEU:HD23	1.88	0.55
1:D:137:TYR:CD2	1:D:291:ASN:HB3	2.41	0.55
1:D:226:TRP:CZ2	1:D:332:GLY:HA2	2.41	0.55
1:B:481:GLN:HA	1:B:488:TYR:CE2	2.42	0.55
1:B:2:GLU:CD	1:B:4:ILE:HG12	2.27	0.55
1:C:9:LYS:O	1:C:57:LYS:HD2	2.05	0.55
1:D:301:ASP:O	1:D:305:ILE:HG13	2.06	0.55
1:D:471:ALA:HB3	1:D:544:LYS:CE	2.34	0.55
1:A:483:ASP:HB2	1:A:485:THR:HG23	1.87	0.55
1:C:168:PRO:HA	1:C:177:VAL:HA	1.87	0.55
1:B:51:GLY:O	1:B:120:GLU:HA	2.07	0.55
1:C:200:GLU:OE1	1:C:200:GLU:HA	2.07	0.55
1:A:472:LEU:CD1	1:A:484:TYR:HB3	2.37	0.55
1:C:305:ILE:HG13	1:C:514:MET:HE2	1.89	0.55
1:A:302:ILE:HD12	1:A:327:LEU:HB3	1.89	0.55
1:D:169:GLU:O	1:D:175:ALA:HA	2.05	0.55
1:C:88:LYS:O	1:C:90:VAL:HG23	2.06	0.54
1:D:230:LYS:N	1:D:230:LYS:CD	2.70	0.54



	so ao pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:280:VAL:HG12	1:D:511:VAL:HG13	1.89	0.54
1:B:536:VAL:HG12	1:B:537:THR:H	1.71	0.54
1:C:316:ALA:HB1	1:C:317:HIS:HA	1.88	0.54
1:D:192:LEU:CD2	1:D:241:LEU:HD22	2.36	0.54
1:B:75:ARG:O	1:B:142:ARG:HD2	2.07	0.54
1:C:302:ILE:HG23	1:C:331:ARG:NH1	2.22	0.54
1:B:536:VAL:HG12	1:B:537:THR:N	2.22	0.54
1:C:443:VAL:HG23	1:C:496:MET:HE1	1.90	0.54
1:C:362:VAL:HG13	4:C:1604:FMN:C6	2.38	0.54
1:C:476:THR:HG22	1:C:485:THR:HG21	1.89	0.54
1:D:60:LYS:HA	1:D:111:GLU:O	2.08	0.54
1:D:283:HIS:HD2	1:D:517:PHE:CD2	2.26	0.54
1:B:367:HIS:HB2	1:B:370:ILE:HD12	1.89	0.54
1:D:277:LEU:O	1:D:508:ALA:HA	2.05	0.54
1:A:517:PHE:CZ	1:A:531:ASN:HB3	2.43	0.54
1:C:282:ARG:HH21	1:C:284:GLN:HA	1.71	0.54
1:C:471:ALA:HB2	1:C:489:GLN:HB2	1.90	0.54
1:C:542:TYR:OH	1:C:566:ARG:HD2	2.08	0.54
1:A:560:VAL:HG21	1:A:621:ALA:HB3	1.89	0.53
1:C:434:HIS:HB2	1:C:464:MET:CE	2.38	0.53
1:D:339:ILE:HD12	1:D:341:TYR:H	1.73	0.53
1:D:583:LEU:HB3	1:D:584:PRO:HD2	1.88	0.53
1:A:192:LEU:O	1:A:208:GLU:HA	2.09	0.53
1:B:168:PRO:CA	1:B:177:VAL:HG12	2.38	0.53
1:C:313:ILE:HB	1:C:335:ILE:CD1	2.39	0.53
1:C:316:ALA:HB1	1:C:317:HIS:ND1	2.23	0.53
1:D:354:ILE:HG23	1:D:399:MET:SD	2.49	0.53
1:B:354:ILE:HG23	1:B:399:MET:CE	2.37	0.53
1:B:615:SER:HB2	1:B:630:ILE:CG1	2.38	0.53
1:C:235:TYR:HB2	1:C:255:PHE:CE1	2.43	0.53
1:D:119:VAL:HG21	1:D:140:LEU:CD1	2.38	0.53
1:D:340:PRO:O	1:D:342:ILE:HG22	2.08	0.53
1:D:386:ASP:O	1:D:390:LEU:HG	2.09	0.53
1:B:174:ASP:OD1	1:B:221:PRO:HA	2.07	0.53
1:C:314:ARG:NH2	1:C:338:GLU:OE1	2.36	0.53
1:D:83:VAL:HG22	1:D:117:ILE:HG12	1.90	0.53
1:C:51:GLY:O	1:C:120:GLU:HA	2.09	0.53
1:C:155:ASP:HA	1:C:184:THR:OG1	2.08	0.53
1:C:278:ARG:HD2	1:C:501:PHE:CD1	2.43	0.53
1:C:55:TYR:CE2	1:C:140:LEU:HG	2.43	0.53
1:C:436:PHE:HB2	1:C:446:ASN:HD21	1.73	0.53



	is us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:727:LEU:HD12	1:C:727:LEU:O	2.09	0.53
1:A:11:ALA:HB3	1:A:56:ALA:HB3	1.89	0.53
1:A:154:PHE:CD2	1:A:251:VAL:HG22	2.44	0.53
1:B:474:TRP:CE2	1:B:642:LEU:HD13	2.44	0.53
1:D:24:PRO:HG2	1:D:27:TRP:CE3	2.44	0.53
1:D:128:TYR:CZ	1:D:346:MET:HE2	2.44	0.53
1:A:598:LEU:HB2	1:A:607:PHE:CE2	2.44	0.53
1:C:37:ASN:HA	1:C:40:ASP:OD1	2.08	0.53
1:D:101:ARG:CD	1:D:156:LEU:HD22	2.39	0.53
1:D:429:VAL:HG12	1:D:461:PRO:CG	2.39	0.53
1:D:472:LEU:HD21	1:D:532:HIS:ND1	2.23	0.53
1:D:497:ILE:HA	1:D:501:PHE:CD1	2.44	0.53
1:D:503:ARG:HB3	1:D:505:TYR:CE2	2.43	0.53
1:A:6:PHE:CE1	1:A:57:LYS:HE2	2.44	0.53
1:D:165:LYS:HB3	1:D:180:GLU:HB2	1.91	0.53
1:A:24:PRO:HG2	1:A:27:TRP:CZ3	2.44	0.52
1:A:217:VAL:HG13	1:A:217:VAL:O	2.09	0.52
1:A:335:ILE:HG12	1:A:369:SER:OG	2.09	0.52
1:A:78:ASN:ND2	1:A:137:TYR:O	2.28	0.52
1:A:432:TYR:HB3	1:A:434:HIS:CD2	2.44	0.52
1:B:583:LEU:HB3	1:B:584:PRO:HD2	1.91	0.52
1:C:618:VAL:HG11	2:C:1602:GOL:H12	1.91	0.52
1:B:453:PHE:HD1	1:B:462:LEU:HD22	1.73	0.52
1:C:424:ILE:HG23	1:C:430:ILE:HD13	1.91	0.52
1:B:444:SER:HA	1:B:499:GLN:HE22	1.74	0.52
1:C:209:THR:HB	1:C:213:GLU:HG2	1.92	0.52
1:C:411:ILE:HD12	1:C:423:TYR:CE2	2.44	0.52
1:A:168:PRO:HA	1:A:177:VAL:HA	1.91	0.52
1:B:474:TRP:CZ2	1:B:642:LEU:HD13	2.45	0.52
1:B:575:THR:HG22	1:B:609:VAL:O	2.10	0.52
1:D:154:PHE:HE2	1:D:239:VAL:HG22	1.73	0.52
1:D:279:GLY:HA3	1:D:312:THR:O	2.10	0.52
1:B:280:VAL:HG21	1:B:305:ILE:CD1	2.39	0.52
1:A:279:GLY:HA3	1:A:312:THR:O	2.10	0.52
1:A:404:ASP:OD2	1:A:407:ARG:HB2	2.10	0.52
1:A:423:TYR:O	1:A:426:ILE:HD12	2.10	0.52
1:A:282:ARG:HD2	1:A:301:ASP:OD2	2.10	0.52
1:D:162:PRO:O	1:D:251:VAL:HG21	2.09	0.52
1:D:126:ARG:HA	1:D:349:GLY:CA	2.40	0.52
1:A:500:LEU:HD23	1:A:509:THR:CG2	2.40	0.51
1:B:59:LEU:HD11	1:B:64:LEU:HD13	1.92	0.51



	is as pagen	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:294:LEU:HB2	1:D:297:HIS:ND1	2.24	0.51
1:B:305:ILE:HD13	1:B:514:MET:CE	2.40	0.51
1:D:164:ILE:HD12	1:D:251:VAL:CG1	2.40	0.51
1:D:165:LYS:HE3	1:D:365:TYR:CE2	2.46	0.51
1:D:443:VAL:HG23	1:D:496:MET:CE	2.37	0.51
1:A:32:LEU:HA	1:A:33:PRO:C	2.31	0.51
1:A:175:ALA:HB2	1:A:223:VAL:CG2	2.41	0.51
1:A:282:ARG:HG2	1:A:283:HIS:O	2.10	0.51
1:A:309:GLY:O	1:A:554:LEU:HB3	2.10	0.51
1:B:83:VAL:O	1:B:90:VAL:HG22	2.09	0.51
1:C:325:TYR:HB3	1:C:367:HIS:CD2	2.44	0.51
1:A:7:ASN:HB3	1:A:32:LEU:HB2	1.91	0.51
1:B:317:HIS:HA	1:B:338:GLU:OE2	2.10	0.51
1:D:340:PRO:HG3	1:D:356:GLN:OE1	2.10	0.51
1:A:158:TYR:HE2	1:A:362:VAL:HG21	1.75	0.51
1:A:372:VAL:HA	1:A:408:LEU:O	2.10	0.51
1:D:284:GLN:HG2	1:D:318:TYR:OH	2.11	0.51
1:D:426:ILE:HD12	1:D:426:ILE:H	1.76	0.51
1:A:562:LEU:HD13	1:A:628:SER:HB2	1.93	0.51
1:B:418:ASP:OD2	1:B:420:HIS:HB2	2.11	0.51
1:B:415:SER:HB2	1:B:433:ASN:O	2.11	0.51
1:D:154:PHE:HE1	1:D:249:ASP:HB2	1.69	0.51
1:D:423:TYR:HA	1:D:426:ILE:HD11	1.91	0.51
1:B:618:VAL:HG22	1:B:627:GLU:HG3	1.93	0.51
1:D:129:PRO:HG3	1:D:340:PRO:HB3	1.93	0.51
1:D:358:LYS:O	1:D:362:VAL:HG23	2.11	0.51
1:A:170:ILE:CD1	1:A:225:LEU:HD21	2.37	0.51
1:A:277:LEU:HD22	1:A:334:VAL:CG2	2.36	0.51
1:B:362:VAL:HG13	4:B:805:FMN:H6	1.93	0.51
1:B:469:CYS:C	1:B:533:LYS:HG2	2.31	0.51
1:C:419:ILE:CG2	1:C:453:PHE:HD2	2.24	0.51
1:D:72:LEU:CD2	1:D:74:LEU:HD11	2.40	0.51
1:D:438:TRP:CE3	1:D:438:TRP:HA	2.46	0.51
1:A:311:THR:O	1:A:334:VAL:HG22	2.11	0.50
1:A:473:ASN:HA	1:A:566:ARG:HH22	1.76	0.50
1:D:137:TYR:HD2	1:D:291:ASN:HB3	1.76	0.50
1:B:316:ALA:HB1	1:B:317:HIS:HA	1.94	0.50
1:D:129:PRO:HD3	1:D:340:PRO:CB	2.41	0.50
1:D:560:VAL:HG21	1:D:621:ALA:HB3	1.92	0.50
1:A:350:ARG:HD2	1:B:17:THR:HG21	1.93	0.50
1:A:568:VAL:HG13	1:A:629:HIS:O	2.11	0.50



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:443:VAL:CG2	1:B:496:MET:HE2	2.40	0.50
1:C:90:VAL:HG12	1:C:102:VAL:HG21	1.92	0.50
1:D:268:PHE:CE2	1:D:270:LEU:HB2	2.46	0.50
1:D:467:TYR:CD2	1:D:496:MET:HG3	2.47	0.50
1:B:38:GLU:HG2	1:B:289:ILE:C	2.32	0.50
1:B:59:LEU:HD11	1:B:64:LEU:CD1	2.42	0.50
1:C:75:ARG:O	1:C:142:ARG:HD2	2.12	0.50
1:C:474:TRP:CZ2	1:C:642:LEU:HD13	2.45	0.50
1:D:373:TRP:O	1:D:409:THR:HA	2.12	0.50
1:A:310:ALA:HA	1:A:554:LEU:HD13	1.93	0.50
1:A:436:PHE:HB2	1:A:446:ASN:OD1	2.11	0.50
1:C:277:LEU:HD22	1:C:312:THR:HB	1.93	0.50
1:C:286:ARG:NH1	1:C:300:GLU:OE1	2.30	0.50
1:C:315:LEU:HD21	1:C:324:PHE:CE2	2.46	0.50
1:D:5:ASN:OD1	1:D:6:PHE:N	2.44	0.50
1:D:32:LEU:CD1	1:D:34:HIS:HB3	2.41	0.50
1:D:230:LYS:HE3	1:D:230:LYS:CA	2.40	0.50
1:B:73:GLU:OE1	1:B:147:ILE:HD11	2.12	0.50
1:A:341:TYR:CE1	1:A:379:ILE:HD11	2.47	0.50
1:A:527:GLU:HB3	1:A:532:HIS:CE1	2.46	0.50
1:D:469:CYS:HB3	1:D:489:GLN:HG2	1.94	0.50
1:B:354:ILE:HG23	1:B:399:MET:HE1	1.92	0.50
1:D:280:VAL:HG12	1:D:511:VAL:HG12	1.90	0.50
1:B:305:ILE:HG21	1:B:313:ILE:HD11	1.94	0.49
1:B:590:VAL:HG12	1:B:617:LEU:CD2	2.42	0.49
1:D:150:ASN:HB2	1:D:248:VAL:HG13	1.93	0.49
1:A:10:TRP:CE2	1:A:57:LYS:HD3	2.47	0.49
1:A:107:GLU:HA	1:A:107:GLU:OE1	2.13	0.49
1:B:13:THR:HG21	1:B:27:TRP:CZ2	2.47	0.49
1:B:380:THR:CG2	1:B:380:THR:O	2.61	0.49
1:A:9:LYS:O	1:A:57:LYS:HD2	2.11	0.49
1:A:535:LEU:O	1:A:544:LYS:HG3	2.11	0.49
1:B:395:ILE:O	1:B:399:MET:HB2	2.12	0.49
1:B:443:VAL:O	1:B:499:GLN:NE2	2.43	0.49
1:C:314:ARG:HA	1:C:336:TRP:HB3	1.94	0.49
1:D:474:TRP:CE2	1:D:642:LEU:HB2	2.47	0.49
1:D:500:LEU:HD23	1:D:509:THR:CG2	2.40	0.49
1:A:402:GLU:O	1:A:402:GLU:HG2	2.12	0.49
1:B:313:ILE:HB	1:B:335:ILE:CD1	2.43	0.49
1:D:20:PRO:HG3	1:D:27:TRP:CH2	2.47	0.49
1:B:360:LEU:O	1:B:364:ASN:ND2	2.32	0.49



	to do pagon	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:617:LEU:HD11	1:B:630:ILE:HG21	1.95	0.49
1:C:438:TRP:CZ2	1:C:470:GLU:HG3	2.48	0.49
1:D:36:TRP:CZ2	1:D:121:ASN:ND2	2.80	0.49
1:D:284:GLN:HG2	1:D:318:TYR:CZ	2.47	0.49
1:A:51:GLY:O	1:A:120:GLU:HA	2.11	0.49
1:A:160:GLY:O	1:A:363:GLN:HG2	2.13	0.49
1:B:413:VAL:CG1	1:B:417:CYS:HB3	2.42	0.49
1:A:284:GLN:HG2	1:A:318:TYR:HE1	1.74	0.49
1:C:262:ILE:CD1	1:C:408:LEU:HD12	2.43	0.49
1:C:450:MET:SD	1:C:462:LEU:HD21	2.52	0.49
1:D:413:VAL:HG12	1:D:414:VAL:O	2.12	0.49
1:A:61:LYS:HE2	1:A:108:LEU:O	2.13	0.49
1:C:196:VAL:HG12	1:C:204:VAL:HG23	1.94	0.49
1:C:389:LEU:O	1:C:389:LEU:HD23	2.12	0.49
1:D:392:ASN:HA	1:D:395:ILE:HD13	1.93	0.49
1:A:233:TYR:O	1:A:234:LEU:HD23	2.13	0.49
1:A:313:ILE:HD11	1:A:333:LEU:HD22	1.94	0.49
1:B:300:GLU:O	1:B:304:LEU:HD12	2.13	0.49
1:C:596:GLY:HA2	1:D:597:LYS:O	2.13	0.49
1:C:613:GLY:O	1:C:631:ARG:HA	2.12	0.49
1:A:415:SER:HB3	1:A:433:ASN:O	2.13	0.49
1:B:493:HIS:O	1:B:497:ILE:HG13	2.13	0.49
1:C:166:VAL:HG11	1:C:255:PHE:CG	2.47	0.49
1:A:473:ASN:CG	1:A:566:ARG:HH21	2.16	0.48
1:B:282:ARG:HG2	1:B:283:HIS:N	2.27	0.48
1:B:431:SER:HB2	1:B:465:SER:OG	2.13	0.48
1:C:280:VAL:HG12	1:C:511:VAL:HB	1.94	0.48
1:C:556:ASP:O	1:C:558:PRO:HD3	2.13	0.48
1:D:493:HIS:O	1:D:497:ILE:HG13	2.13	0.48
1:B:531:ASN:HD21	3:B:804:BDP:C6	2.26	0.48
1:C:440:GLY:N	1:C:719:PHE:HE1	2.11	0.48
1:D:589:PHE:HD1	1:D:594:SER:HA	1.76	0.48
1:A:168:PRO:HB3	1:A:177:VAL:CG1	2.42	0.48
1:A:204:VAL:HG12	1:A:204:VAL:O	2.12	0.48
1:A:473:ASN:OD1	1:A:566:ARG:NH2	2.46	0.48
1:D:497:ILE:HG23	1:D:501:PHE:CD1	2.49	0.48
1:A:37:ASN:HA	1:A:40:ASP:OD1	2.12	0.48
1:A:175:ALA:HB2	1:A:223:VAL:HG21	1.95	0.48
1:C:372:VAL:HA	1:C:408:LEU:O	2.13	0.48
1:C:399:MET:O	1:C:403:MET:HG3	2.13	0.48
1:D:429:VAL:HG12	1:D:461:PRO:CB	2.43	0.48



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:223:VAL:HG13	1:C:225:LEU:CD2	2.43	0.48
1:D:13:THR:HG21	1:D:27:TRP:CZ2	2.48	0.48
1:A:293:LEU:HD23	1:A:298:HIS:CE1	2.49	0.48
1:B:18:GLU:O	1:B:18:GLU:HG3	2.12	0.48
1:B:88:LYS:O	1:B:90:VAL:HG13	2.13	0.48
1:D:181:VAL:HG11	1:D:239:VAL:HG21	1.96	0.48
1:A:558:PRO:HB2	1:A:624:TYR:CZ	2.48	0.48
1:B:127:VAL:O	1:B:130:GLN:HG2	2.14	0.48
1:D:280:VAL:O	1:D:313:ILE:HA	2.13	0.48
1:C:154:PHE:HE2	1:C:250:ALA:HA	1.77	0.48
1:C:305:ILE:HD13	1:C:313:ILE:CD1	2.42	0.48
1:A:175:ALA:HB3	1:A:220:ILE:HG23	1.95	0.48
1:B:590:VAL:CG1	1:B:609:VAL:HG21	2.44	0.48
1:C:720:THR:HG22	1:C:723:ARG:HB3	1.96	0.48
1:A:112:GLU:OE1	1:A:112:GLU:N	2.46	0.48
1:D:573:ASP:O	1:D:611:ASN:N	2.33	0.48
1:B:411:ILE:HG23	1:B:427:PRO:HG3	1.94	0.47
1:C:181:VAL:HG11	1:C:239:VAL:HG11	1.95	0.47
1:D:411:ILE:CD1	1:D:413:VAL:HG23	2.44	0.47
1:D:483:ASP:HB2	1:D:485:THR:HG23	1.95	0.47
1:B:380:THR:O	1:B:380:THR:HG22	2.14	0.47
1:C:278:ARG:HD3	1:C:509:THR:HG23	1.94	0.47
1:D:150:ASN:OD1	1:D:151:LYS:N	2.48	0.47
1:D:230:LYS:HD2	1:D:230:LYS:H	1.75	0.47
1:D:438:TRP:HE1	1:D:470:GLU:HG3	1.79	0.47
1:C:83:VAL:HG22	1:C:117:ILE:HG12	1.96	0.47
1:C:591:ASN:OD1	1:C:615:SER:HA	2.15	0.47
1:C:611:ASN:O	1:C:632:LYS:HD3	2.15	0.47
1:A:411:ILE:HD12	1:A:413:VAL:HG23	1.96	0.47
1:A:470:GLU:HG2	1:A:533:LYS:CG	2.44	0.47
1:C:101:ARG:HH21	1:C:156:LEU:CA	2.22	0.47
1:C:522:ARG:NH1	1:C:524:GLU:OE2	2.41	0.47
1:D:614:GLU:HG2	1:D:631:ARG:CB	2.44	0.47
1:A:84:TYR:HA	1:A:88:LYS:O	2.15	0.47
1:B:162:PRO:O	1:B:251:VAL:HG21	2.14	0.47
1:D:478:ASP:OD2	1:D:480:LYS:HE3	2.14	0.47
1:D:587:GLU:HB3	1:D:620:VAL:CG2	2.44	0.47
1:A:194:TYR:HB2	1:A:207:THR:HG22	1.95	0.47
1:A:232:PRO:HB3	1:A:332:GLY:CA	2.45	0.47
1:A:277:LEU:O	1:A:508:ALA:HA	2.14	0.47
1:B:68:ASP:O	1:B:105:THR:HG21	2.15	0.47



	lo uo pugo	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:584:PRO:O	1:B:599:GLN:HG2	2.14	0.47
1:C:180:GLU:HA	1:C:214:THR:O	2.14	0.47
1:D:259:THR:OG1	1:D:271:ASN:HA	2.14	0.47
1:D:270:LEU:HD23	1:D:275:TYR:CD2	2.50	0.47
1:A:59:LEU:HD23	1:A:59:LEU:C	2.35	0.47
1:B:466:GLU:OE1	3:B:804:BDP:H1	2.15	0.47
1:B:549:ALA:HB2	1:B:580:TYR:CE2	2.50	0.47
1:C:590:VAL:HG13	1:C:590:VAL:O	2.15	0.47
1:D:372:VAL:HG23	1:D:372:VAL:O	2.15	0.47
1:A:90:VAL:HG12	1:A:102:VAL:HG21	1.97	0.47
1:A:189:ASP:OD1	1:A:189:ASP:N	2.47	0.47
1:A:198:ASP:OD1	1:A:200:GLU:HG2	2.14	0.47
1:A:376:SER:HB3	1:A:393:HIS:NE2	2.30	0.47
1:B:315:LEU:HD12	1:B:325:TYR:CE1	2.49	0.47
1:C:16:ALA:HB3	1:C:54:TYR:CD1	2.50	0.47
1:C:367:HIS:HB2	1:C:370:ILE:CD1	2.31	0.47
1:C:501:PHE:HE2	1:C:554:LEU:HD21	1.78	0.47
1:D:364:ASN:HB2	1:D:373:TRP:HH2	1.80	0.47
1:B:512:TRP:HA	1:B:513:ASN:HA	1.76	0.47
1:C:73:GLU:HB2	1:C:147:ILE:CD1	2.44	0.47
1:C:81:ALA:HA	1:C:118:ALA:O	2.14	0.47
1:D:248:VAL:HG12	1:D:249:ASP:N	2.29	0.47
1:A:81:ALA:HA	1:A:118:ALA:O	2.14	0.46
1:A:470:GLU:HG2	1:A:533:LYS:HG2	1.97	0.46
1:B:74:LEU:HD21	1:B:117:ILE:HD13	1.97	0.46
1:B:111:GLU:CG	1:B:111:GLU:O	2.62	0.46
1:D:623:GLU:O	1:D:623:GLU:CG	2.61	0.46
1:A:312:THR:CB	1:A:334:VAL:HG23	2.45	0.46
1:A:519:ALA:HB3	1:A:522:ARG:HG3	1.97	0.46
1:C:433:ASN:CG	1:C:466:GLU:HB2	2.36	0.46
1:D:192:LEU:HD12	1:D:211:ALA:O	2.14	0.46
1:D:464:MET:HG2	1:D:500:LEU:HD21	1.96	0.46
1:A:588:LEU:HD21	1:A:609:VAL:HG21	1.97	0.46
1:B:58:GLN:HG2	1:B:114:LEU:CD1	2.45	0.46
1:D:165:LYS:HE3	1:D:365:TYR:CZ	2.50	0.46
1:B:40:ASP:HA	1:B:43:ASP:OD2	2.15	0.46
1:B:110:GLU:C	1:B:112:GLU:H	2.18	0.46
1:D:286:ARG:HB3	1:D:289:ILE:HD11	1.97	0.46
1:A:494:GLU:HG2	1:A:604:PHE:CE2	2.51	0.46
1:A:562:LEU:HD23	1:A:562:LEU:HA	1.76	0.46
1:B:68:ASP:OD2	1:B:151:LYS:HG2	2.15	0.46



	ti a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:617:LEU:HD12	1:B:628:SER:OG	2.15	0.46
1:C:24:PRO:HG2	1:C:27:TRP:CE3	2.50	0.46
1:D:236:THR:HG22	1:D:254:ARG:HG2	1.97	0.46
1:A:497:ILE:HD12	1:A:604:PHE:CZ	2.46	0.46
1:B:474:TRP:O	1:B:485:THR:HB	2.14	0.46
1:C:23:MET:SD	1:C:24:PRO:HD2	2.56	0.46
1:C:171:LYS:HE2	1:C:176:SER:OG	2.15	0.46
1:C:262:ILE:HD12	1:C:408:LEU:CD1	2.46	0.46
1:C:125:ASP:HA	1:C:346:MET:SD	2.55	0.46
1:D:395:ILE:HD12	1:D:395:ILE:N	2.19	0.46
1:D:611:ASN:OD1	1:D:630:ILE:HD12	2.16	0.46
1:B:421:ASP:OD1	1:B:422:PRO:HD2	2.16	0.46
1:B:588:LEU:HD11	1:B:617:LEU:HB3	1.97	0.46
4:C:1604:FMN:O2'	4:C:1604:FMN:H9	2.15	0.46
1:D:10:TRP:CE2	1:D:57:LYS:HD2	2.51	0.46
1:D:225:LEU:H	1:D:225:LEU:CD2	2.26	0.46
1:D:477:SER:O	1:D:479:PRO:HD3	2.16	0.46
1:A:619:ALA:O	1:A:625:LYS:HA	2.16	0.46
1:B:372:VAL:HA	1:B:408:LEU:O	2.15	0.46
1:B:475:HIS:HA	1:B:487:GLU:OE1	2.16	0.46
1:B:562:LEU:HD21	1:B:619:ALA:CB	2.46	0.46
1:D:164:ILE:HD11	1:D:239:VAL:CG1	2.45	0.46
1:D:289:ILE:HD12	1:D:293:LEU:HD12	1.97	0.46
1:A:75:ARG:O	1:A:142:ARG:HD2	2.16	0.46
1:A:329:ASP:OD1	1:A:369:SER:HB3	2.16	0.46
1:A:411:ILE:CD1	1:A:413:VAL:HG23	2.46	0.46
1:B:436:PHE:HB2	1:B:446:ASN:OD1	2.16	0.46
1:C:209:THR:CB	1:C:213:GLU:HG2	2.46	0.46
1:D:24:PRO:HG2	1:D:27:TRP:CZ3	2.51	0.46
1:D:101:ARG:HD2	1:D:156:LEU:HD22	1.98	0.46
1:B:360:LEU:HD12	1:B:364:ASN:ND2	2.30	0.45
1:B:481:GLN:HB2	1:B:488:TYR:OH	2.15	0.45
1:D:269:ILE:HG23	1:D:273:GLU:O	2.16	0.45
1:A:226:TRP:CZ2	1:A:332:GLY:HA2	2.50	0.45
1:D:424:ILE:HG23	1:D:430:ILE:HD13	1.98	0.45
1:D:453:PHE:CD1	1:D:462:LEU:HD13	2.51	0.45
1:D:539:ASP:CG	1:D:541:LYS:HB2	2.35	0.45
1:A:411:ILE:HG12	1:A:427:PRO:HG3	1.97	0.45
1:B:270:LEU:HD23	1:B:275:TYR:CD2	2.51	0.45
1:C:493:HIS:CE1	1:C:511:VAL:HG13	2.50	0.45
1:D:193:VAL:HG22	1:D:240:ALA:HB3	1.98	0.45



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:503:ARG:HG3	1:D:503:ARG:HH11	1.82	0.45
1:A:191:LYS:HD2	1:A:208:GLU:OE2	2.17	0.45
1:C:196:VAL:HG12	1:C:204:VAL:CG2	2.47	0.45
1:C:282:ARG:O	1:C:282:ARG:HG3	2.17	0.45
1:D:373:TRP:HE1	1:D:407:ARG:HD2	1.81	0.45
1:D:336:TRP:CD1	1:D:336:TRP:C	2.89	0.45
1:A:515:PHE:HD1	1:A:536:VAL:HB	1.82	0.45
1:A:560:VAL:HG21	1:A:621:ALA:CB	2.47	0.45
1:C:58:GLN:HE21	1:C:112:GLU:HB3	1.81	0.45
1:D:336:TRP:HB2	1:D:372:VAL:CG2	2.47	0.45
1:D:407:ARG:C	1:D:408:LEU:HD23	2.36	0.45
1:A:426:ILE:HB	1:A:427:PRO:HD3	1.98	0.45
1:C:385:SER:OG	1:C:421:ASP:OD1	2.33	0.45
1:C:249:ASP:OD1	1:C:250:ALA:N	2.46	0.45
1:D:395:ILE:H	1:D:395:ILE:CD1	2.15	0.45
1:B:220:ILE:CG2	1:B:223:VAL:HG12	2.48	0.45
1:C:196:VAL:CG1	1:C:220:ILE:HD11	2.39	0.45
1:D:277:LEU:CD1	1:D:334:VAL:HG11	2.46	0.45
1:A:270:LEU:HD23	1:A:271:ASN:N	2.32	0.44
1:C:305:ILE:HG13	1:C:514:MET:CE	2.46	0.44
1:C:315:LEU:HD12	1:C:325:TYR:CE1	2.52	0.44
1:D:126:ARG:HA	1:D:349:GLY:HA3	1.98	0.44
1:D:411:ILE:HG12	1:D:427:PRO:HG3	1.99	0.44
1:A:238:GLU:HG2	1:A:252:SER:HB2	1.99	0.44
1:B:438:TRP:CE2	1:B:470:GLU:HG3	2.51	0.44
1:B:457:PHE:HB3	1:B:460:ILE:HG13	1.99	0.44
1:B:576:LYS:HB3	1:B:576:LYS:HE2	1.77	0.44
1:A:223:VAL:CG1	1:A:225:LEU:HD23	2.47	0.44
1:A:312:THR:HB	1:A:334:VAL:CG2	2.47	0.44
1:B:391:GLU:OE2	1:B:394:ARG:NH2	2.48	0.44
1:B:493:HIS:HA	1:B:496:MET:HB2	1.99	0.44
1:B:617:LEU:HD11	1:B:630:ILE:CG2	2.47	0.44
1:C:1:ARG:HD3	1:C:249:ASP:OD1	2.17	0.44
1:D:457:PHE:N	1:D:457:PHE:CD1	2.84	0.44
1:A:191:LYS:HA	1:A:210:ALA:HA	2.00	0.44
1:A:371:VAL:HA	1:A:407:ARG:HG2	1.98	0.44
1:A:414:VAL:HG22	1:A:416:MET:H	1.81	0.44
1:B:19:VAL:HG13	1:B:116:VAL:HG21	2.00	0.44
1:B:282:ARG:HG2	1:B:283:HIS:O	2.17	0.44
1:C:32:LEU:HA	1:C:33:PRO:C	2.37	0.44
1:C:719:PHE:HB3	1:C:723:ARG:HG2	1.99	0.44



	so ao pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:226:TRP:O	1:D:271:ASN:ND2	2.51	0.44
1:A:254:ARG:HE	1:A:254:ARG:HB2	1.59	0.44
1:A:483:ASP:CB	1:A:485:THR:HG23	2.48	0.44
1:B:137:TYR:CD2	1:B:291:ASN:HB3	2.52	0.44
1:B:220:ILE:O	1:B:223:VAL:HG13	2.17	0.44
1:C:198:ASP:HB3	1:C:202:LYS:HB2	1.99	0.44
1:D:141:TYR:HD1	1:D:141:TYR:H	1.65	0.44
1:D:338:GLU:O	1:D:360:LEU:HD22	2.18	0.44
1:A:492:TYR:O	1:A:496:MET:HG2	2.18	0.44
1:B:557:GLU:OE1	1:B:557:GLU:HA	2.17	0.44
1:C:260:PHE:HA	1:C:269:ILE:O	2.18	0.44
1:C:312:THR:HA	1:C:334:VAL:O	2.18	0.44
1:C:424:ILE:HG22	1:C:424:ILE:O	2.18	0.44
1:C:530:GLN:HE21	1:C:538:PHE:CB	2.29	0.44
1:A:73:GLU:HB2	1:A:147:ILE:CD1	2.45	0.44
1:A:76:GLY:HA3	1:A:142:ARG:HG3	1.99	0.44
1:A:544:LYS:O	1:A:547:PHE:HB3	2.18	0.44
1:B:175:ALA:CB	1:B:223:VAL:HG11	2.32	0.44
1:D:11:ALA:HB3	1:D:56:ALA:HB3	2.00	0.44
1:D:32:LEU:HD22	1:D:32:LEU:H	1.83	0.44
1:B:175:ALA:HB3	1:B:223:VAL:CG1	2.35	0.44
1:C:530:GLN:HB3	1:C:532:HIS:NE2	2.31	0.44
1:D:270:LEU:HD23	1:D:275:TYR:HD2	1.83	0.44
1:D:366:ASN:O	1:D:368:PRO:HD3	2.18	0.44
1:D:614:GLU:HG2	1:D:631:ARG:HB3	1.99	0.44
1:A:195:THR:CG2	1:A:238:GLU:HB2	2.46	0.44
1:A:429:VAL:HG21	1:A:507:TRP:CZ2	2.52	0.44
1:A:531:ASN:OD1	1:A:533:LYS:HB2	2.18	0.44
1:A:598:LEU:HB2	1:A:607:PHE:CZ	2.53	0.44
1:C:418:ASP:OD1	1:C:419:ILE:N	2.51	0.44
1:C:438:TRP:O	1:C:723:ARG:NH2	2.51	0.44
1:D:339:ILE:HD12	1:D:341:TYR:HB2	2.00	0.44
1:D:429:VAL:HG12	1:D:461:PRO:HG2	1.99	0.44
1:D:522:ARG:HD2	1:D:524:GLU:OE2	2.16	0.44
1:A:339:ILE:HB	1:A:340:PRO:HD2	2.00	0.43
1:A:460:ILE:HD13	1:A:460:ILE:HA	1.82	0.43
1:B:68:ASP:HB3	1:B:151:LYS:HG2	1.98	0.43
1:C:450:MET:CE	1:C:462:LEU:HG	2.48	0.43
1:C:519:ALA:HB1	2:C:1603:GOL:O1	2.17	0.43
1:D:572:GLU:O	1:D:572:GLU:HG2	2.18	0.43
1:A:20:PRO:HG3	1:A:27:TRP:CH2	2.53	0.43



		Interatomic Clash		
Atom-1	Atom-2	distance $(Å)$	overlap (Å)	
1:C:404:ASP:OD2	1:C:407:ARG:HG3	2.18	0.43	
1:D:93:HIS:NE2	1:D:95:GLY:O	2.48	0.43	
1:D:192:LEU:HD12	1:D:212:GLY:HA2	2.01	0.43	
1:A:170:ILE:HD12	1:A:259:THR:HG23	1.99	0.43	
1:B:111:GLU:O	1:B:111:GLU:HG3	2.19	0.43	
1:B:234:LEU:HD11	1:B:329:ASP:O	2.17	0.43	
1:B:278:ARG:HD2	1:B:501:PHE:CE1	2.53	0.43	
1:B:568:VAL:HG23	1:B:569:ASP:N	2.33	0.43	
1:C:202:LYS:HD3	1:C:202:LYS:HA	1.75	0.43	
1:A:552:ALA:HB1	1:A:603:HIS:HB3	1.99	0.43	
1:B:78:ASN:HA	1:B:79:ALA:HA	1.63	0.43	
1:B:277:LEU:HD11	1:B:334:VAL:HG11	2.01	0.43	
1:B:322:GLN:NE2	1:B:322:GLN:HA	2.34	0.43	
1:B:335:ILE:HD13	1:B:335:ILE:HA	1.81	0.43	
1:C:315:LEU:HD21	1:C:324:PHE:HE2	1.83	0.43	
1:C:569:ASP:OD1	1:C:631:ARG:NH1	2.51	0.43	
1:C:625:LYS:NZ	2:C:1602:GOL:H2	2.34	0.43	
1:D:260:PHE:HA	1:D:269:ILE:O	2.19	0.43	
1:D:436:PHE:HB2	1:D:446:ASN:ND2	2.33	0.43	
1:D:472:LEU:HD21	1:D:532:HIS:CG	2.54	0.43	
1:D:587:GLU:HA	1:D:596:GLY:O	2.18	0.43	
1:A:494:GLU:HG2	1:A:604:PHE:CD2	2.53	0.43	
1:A:500:LEU:HD23	1:A:509:THR:HG21	2.01	0.43	
1:B:494:GLU:OE2	1:B:580:TYR:OH	2.26	0.43	
1:D:129:PRO:HD3	1:D:340:PRO:HB3	1.99	0.43	
1:D:560:VAL:CG2	1:D:621:ALA:HB3	2.48	0.43	
1:A:164:ILE:HD11	1:A:239:VAL:CG2	2.48	0.43	
1:A:442:ASP:H	1:A:445:MET:HE3	1.84	0.43	
1:B:220:ILE:CB	1:B:223:VAL:HG12	2.43	0.43	
1:B:336:TRP:CD1	1:B:336:TRP:C	2.92	0.43	
1:B:527:GLU:HB3	1:B:532:HIS:CE1	2.53	0.43	
1:D:438:TRP:HZ3	1:D:482:GLY:H	1.67	0.43	
1:D:443:VAL:CG2	1:D:495:GLU:HB2	2.47	0.43	
1:D:470:GLU:HA	1:D:532:HIS:O	2.19	0.43	
1:A:471:ALA:HB2	1:A:489:GLN:CB	2.45	0.43	
1:A:512:TRP:HA	1:A:513:ASN:HA	1.70	0.43	
1:C:196:VAL:HG23	1:C:218:LEU:HD13	2.01	0.43	
1:D:81:ALA:HA	1:D:118:ALA:O	2.19	0.43	
1:D:235:TYR:HB3	1:D:255:PHE:CZ	2.53	0.43	
1:B:42:GLN:NE2	1:B:290:GLY:HA2	2.32	0.43	
1:B:168:PRO:HA	1:B:177:VAL:HG12	1.99	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:346:MET:HE2	1:B:346:MET:HB2	1.95	0.43	
1:B:481:GLN:HB2	1:B:488:TYR:CZ	2.53	0.43	
1:D:387:GLU:OE1	1:D:387:GLU:HA	2.18	0.43	
1:D:426:ILE:HB	1:D:427:PRO:HD3	2.01	0.43	
1:D:497:ILE:O	1:D:501:PHE:HB2	2.18	0.43	
1:A:85:VAL:HG22	1:A:115:ILE:HD12	2.00	0.43	
1:A:335:ILE:HD13	1:A:335:ILE:HA	1.83	0.43	
1:C:720:THR:CG2	1:C:723:ARG:H	2.32	0.43	
1:A:129:PRO:HG2	1:A:136:PHE:CE1	2.54	0.43	
1:A:280:VAL:HG21	1:A:514:MET:HB2	2.01	0.43	
1:A:413:VAL:HG11	1:A:432:TYR:CZ	2.54	0.43	
1:B:533:LYS:NZ	3:B:804:BDP:O6A	2.50	0.43	
1:C:12:PHE:CZ	1:C:36:TRP:HB3	2.54	0.43	
1:C:41:GLY:HA2	1:C:48:TYR:HB3	2.01	0.43	
1:C:560:VAL:HG21	1:C:621:ALA:HB3	2.00	0.43	
1:C:581:SER:OG	1:C:583:LEU:HB2	2.18	0.43	
1:A:78:ASN:HA	1:A:79:ALA:HA	1.64	0.42	
1:A:446:ASN:HD22	1:A:464:MET:HE3	1.83	0.42	
1:A:497:ILE:HG23	1:A:501:PHE:CD1	2.53	0.42	
1:B:590:VAL:HG11	1:B:609:VAL:HG21	2.01	0.42	
1:C:426:ILE:N	1:C:427:PRO:HD2	2.34	0.42	
1:D:183:LEU:CD2	1:D:241:LEU:HD11	2.48	0.42	
1:D:428:ASP:OD1	1:D:428:ASP:N	2.50	0.42	
1:A:90:VAL:HG12	1:A:102:VAL:CG2	2.49	0.42	
1:A:154:PHE:CE2	1:A:251:VAL:HG22	2.54	0.42	
1:A:373:TRP:NE1	1:A:407:ARG:HD2	2.34	0.42	
1:B:59:LEU:HD12	1:B:60:LYS:N	2.34	0.42	
1:C:78:ASN:HA	1:C:79:ALA:HA	1.64	0.42	
1:C:521:ALA:HB2	2:C:1603:GOL:O2	2.19	0.42	
1:A:413:VAL:CG1	1:A:417:CYS:HB3	2.49	0.42	
1:D:467:TYR:HD2	1:D:496:MET:HG3	1.84	0.42	
1:A:277:LEU:HD13	1:A:334:VAL:HG21	2.01	0.42	
1:A:424:ILE:HG22	1:A:424:ILE:O	2.19	0.42	
1:C:719:PHE:CD1	1:C:719:PHE:N	2.85	0.42	
1:D:408:LEU:HD23	1:D:408:LEU:N	2.34	0.42	
1:A:400:VAL:HG11	1:A:409:THR:HG22	2.01	0.42	
1:A:424:ILE:HG23	1:A:430:ILE:HD13	2.01	0.42	
1:B:177:VAL:HG23	1:B:177:VAL:O	2.19	0.42	
1:C:133:ASP:O	1:C:517:PHE:HE2	2.02	0.42	
1:D:91:ALA:HB2	1:D:102:VAL:HG11	2.01	0.42	
1:D:587:GLU:O	1:D:620:VAL:HG22	2.18	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:C:432:TYR:HB3	1:C:434:HIS:CD2	2.54	0.42	
1:C:527:GLU:HB3	1:C:532:HIS:CE1	2.54	0.42	
1:A:170:ILE:HD12	1:A:259:THR:CG2	2.50	0.42	
1:A:515:PHE:CD1	1:A:536:VAL:HB	2.55	0.42	
1:C:1:ARG:HD2	1:C:149:VAL:HG12	2.01	0.42	
1:C:78:ASN:CA	1:C:96:GLY:HA3	2.48	0.42	
1:C:361:VAL:O	1:C:365:TYR:HB2	2.20	0.42	
1:D:150:ASN:CB	1:D:248:VAL:HG13	2.50	0.42	
1:D:225:LEU:HD23	1:D:225:LEU:N	2.29	0.42	
1:D:457:PHE:HD1	1:D:457:PHE:N	2.17	0.42	
1:B:181:VAL:O	1:B:214:THR:HB	2.20	0.42	
1:B:413:VAL:HG12	1:B:414:VAL:O	2.18	0.42	
1:D:74:LEU:HG	1:D:144:VAL:HG22	2.00	0.42	
1:A:74:LEU:HD22	1:A:100:TRP:CZ2	2.54	0.42	
1:A:466:GLU:OE1	3:A:802:BDP:H1	2.19	0.42	
1:B:469:CYS:HB3	1:B:489:GLN:HG3	2.00	0.42	
1:B:551:LYS:HD3	1:B:559:PHE:CD2	2.54	0.42	
1:C:170:ILE:N	1:C:170:ILE:HD13	2.35	0.42	
1:C:269:ILE:HD13	1:C:274:GLU:HA	2.02	0.42	
1:C:604:PHE:CD1	1:C:604:PHE:N	2.88	0.42	
1:D:264:PRO:HD3	1:D:461:PRO:HG3	2.02	0.42	
1:B:74:LEU:HD12	1:B:74:LEU:N	2.35	0.42	
1:C:277:LEU:O	1:C:508:ALA:HA	2.20	0.42	
1:C:619:ALA:O	1:C:625:LYS:HA	2.20	0.42	
1:D:94:ASP:HB3	1:D:127:VAL:HG13	2.01	0.42	
1:C:534:GLY:O	1:C:544:LYS:HD2	2.19	0.41	
1:D:12:PHE:CZ	1:D:36:TRP:HB3	2.54	0.41	
1:A:335:ILE:HG12	1:A:369:SER:HG	1.85	0.41	
1:A:336:TRP:C	1:A:336:TRP:CD1	2.93	0.41	
1:B:474:TRP:CH2	2:B:803:GOL:H32	2.56	0.41	
1:C:1:ARG:HD2	1:C:149:VAL:CG1	2.50	0.41	
1:C:7:ASN:CG	1:C:32:LEU:HB2	2.39	0.41	
1:C:336:TRP:CD1	1:C:336:TRP:C	2.93	0.41	
1:A:512:TRP:NE1	3:A:802:BDP:H5	2.36	0.41	
1:B:493:HIS:HE1	1:B:511:VAL:HG23	1.86	0.41	
1:B:504:LYS:O	1:B:504:LYS:HG2	2.20	0.41	
1:C:326:ASP:O	1:C:330:GLU:HG3	2.20	0.41	
1:C:450:MET:HE1	1:C:462:LEU:HG	2.02	0.41	
1:C:611:ASN:ND2	1:C:632:LYS:HD2	2.34	0.41	
1:C:617:LEU:HD11	1:C:630:ILE:CG2	2.51	0.41	
1:D:190:GLN:OE1	1:D:192:LEU:HD11	2.20	0.41	



	is as pagen	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:192:LEU:HA	1:D:240:ALA:O	2.20	0.41	
1:D:265:GLU:OE1	1:D:265:GLU:HA	2.19	0.41	
1:D:345:HIS:CE1	1:D:389:LEU:HA	2.55	0.41	
1:A:227:ASN:OD1	1:A:270:LEU:HD22	2.20	0.41	
1:A:467:TYR:OH	1:A:511:VAL:HG22	2.20	0.41	
1:C:73:GLU:HB3	1:C:145:ASN:HB2	2.02	0.41	
1:C:562:LEU:HD23	1:C:579:VAL:HG22	2.03	0.41	
1:D:32:LEU:HD12	1:D:34:HIS:HB3	2.01	0.41	
1:D:33:PRO:CB	1:D:292:ALA:HB1	2.49	0.41	
1:D:312:THR:HA	1:D:334:VAL:O	2.19	0.41	
1:B:419:ILE:CG2	1:B:453:PHE:HD2	2.33	0.41	
1:C:147:ILE:HG22	1:C:149:VAL:HG13	2.02	0.41	
1:C:343:SER:O	1:C:379:ILE:HD12	2.21	0.41	
1:C:414:VAL:HG13	1:C:417:CYS:HB2	2.03	0.41	
1:D:265:GLU:C	1:D:267:GLY:H	2.24	0.41	
1:D:469:CYS:HB3	1:D:489:GLN:HG3	2.01	0.41	
1:D:533:LYS:HE3	3:D:801:BDP:O6B	2.20	0.41	
1:A:314:ARG:NH1	1:A:466:GLU:HG3	2.36	0.41	
1:A:472:LEU:HB2	1:A:474:TRP:CD1	2.55	0.41	
1:B:181:VAL:CG1	1:B:182:PHE:N	2.83	0.41	
1:C:521:ALA:CB	2:C:1603:GOL:H2	2.51	0.41	
1:A:341:TYR:CD1	1:A:379:ILE:HD11	2.56	0.41	
1:C:339:ILE:HB	1:C:340:PRO:HD2	2.03	0.41	
1:C:410:THR:OG1	1:C:411:ILE:N	2.54	0.41	
1:C:426:ILE:N	1:C:427:PRO:CD	2.84	0.41	
1:A:302:ILE:HD13	1:A:327:LEU:HB3	2.02	0.41	
1:B:277:LEU:O	1:B:508:ALA:HA	2.20	0.41	
1:C:64:LEU:HD12	1:C:64:LEU:HA	1.83	0.41	
1:C:335:ILE:HD13	1:C:335:ILE:HA	1.88	0.41	
1:C:339:ILE:HD13	1:C:357:MET:HE2	2.03	0.41	
1:A:268:PHE:CG	1:A:277:LEU:HG	2.56	0.41	
1:A:497:ILE:HG13	1:A:497:ILE:H	1.63	0.41	
1:B:426:ILE:HB	1:B:427:PRO:HD3	2.01	0.41	
1:C:10:TRP:CE3	1:C:55:TYR:HB3	2.55	0.41	
1:C:58:GLN:NE2	1:C:112:GLU:HB3	2.35	0.41	
1:C:170:ILE:HD11	1:C:257:CYS:HB3	2.02	0.41	
1:C:198:ASP:HB3	1:C:202:LYS:H	1.86	0.41	
1:C:416:MET:HE3	1:C:416:MET:HB3	1.91	0.41	
1:C:512:TRP:HA	1:C:513:ASN:HA	1.78	0.41	
1:C:530:GLN:NE2	1:C:538:PHE:CB	2.76	0.41	
1:C:730:ALA:HB3	5:C:1601:ZG5:C22	2.51	0.41	



	io ao pago	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:213:GLU:H	1:D:213:GLU:HG2	1.61	0.41	
1:A:562:LEU:CD1	1:A:628:SER:HB2	2.50	0.41	
1:B:315:LEU:HB3	1:B:320:HIS:CD2	2.56	0.41	
1:B:496:MET:O	1:B:500:LEU:HG	2.21	0.41	
1:C:64:LEU:HD12	1:C:65:PRO:HD2	2.03	0.41	
1:C:340:PRO:O	1:C:342:ILE:HG22	2.20	0.41	
1:D:83:VAL:O	1:D:90:VAL:HG12	2.21	0.41	
1:D:193:VAL:O	1:D:239:VAL:HA	2.21	0.41	
1:D:305:ILE:HD12	1:D:313:ILE:HD13	2.03	0.41	
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.89	0.40	
1:A:274:GLU:OE1	1:A:504:LYS:NZ	2.44	0.40	
1:B:411:ILE:CG2	1:B:427:PRO:HG3	2.51	0.40	
1:B:619:ALA:O	1:B:625:LYS:HA	2.21	0.40	
1:C:354:ILE:HG23	1:C:399:MET:SD	2.61	0.40	
1:C:389:LEU:HD23	1:C:389:LEU:C	2.41	0.40	
1:A:315:LEU:HD12	1:A:325:TYR:CE1	2.56	0.40	
1:A:364:ASN:HA	1:A:367:HIS:HD2	1.85	0.40	
1:A:611:ASN:HD21	1:A:632:LYS:HA	1.87	0.40	
1:B:365:TYR:CE2	1:B:404:ASP:OD1	2.75	0.40	
1:B:494:GLU:HG2	1:B:604:PHE:CE2	2.55	0.40	
1:C:284:GLN:HG2	1:C:318:TYR:OH	2.22	0.40	
1:C:291:ASN:OD1	1:C:291:ASN:N	2.54	0.40	
1:B:41:GLY:HA3	1:B:135:THR:HG21	2.04	0.40	
1:B:280:VAL:O	1:B:313:ILE:HA	2.21	0.40	
1:B:494:GLU:HG2	1:B:604:PHE:CD2	2.56	0.40	
1:D:6:PHE:HB3	1:D:144:VAL:O	2.22	0.40	
1:D:226:TRP:N	1:D:257:CYS:O	2.41	0.40	
1:A:590:VAL:HG22	1:A:617:LEU:HD22	2.03	0.40	
1:B:110:GLU:O	1:B:113:ASN:ND2	2.54	0.40	
1:C:167:THR:O	1:C:167:THR:OG1	2.34	0.40	
1:C:463:GLY:HA2	1:C:506:ILE:HG23	2.02	0.40	
1:D:590:VAL:HG13	1:D:590:VAL:O	2.21	0.40	
1:B:33:PRO:HB3	1:B:141:TYR:O	2.21	0.40	
1:B:209:THR:HB	1:B:213:GLU:CD	2.42	0.40	
1:B:560:VAL:O	1:B:626:ASP:HB2	2.22	0.40	
1:B:590:VAL:HG11	1:B:609:VAL:CG2	2.51	0.40	
1:B:591:ASN:HD21	1:B:615:SER:HA	1.86	0.40	
1:C:213:GLU:HG3	1:C:215:LYS:O	2.21	0.40	
1:C:549:ALA:HB2	1:C:580:TYR:CE2	2.56	0.40	
1:C:586:VAL:HG22	1:C:621:ALA:HB2	2.04	0.40	
1:D:99:THR:O	1:D:160:GLY:HA3	2.22	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:GLU:HB3	1:D:414:VAL:HB	2.03	0.40
1:D:571:VAL:HG22	1:D:633:VAL:HG23	2.04	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	631/757~(83%)	581 (92%)	49 (8%)	1 (0%)	47	78
1	В	642/757~(85%)	596 (93%)	43 (7%)	3~(0%)	29	61
1	С	653/757~(86%)	609 (93%)	44 (7%)	0	100	100
1	D	605/757~(80%)	545 (90%)	59 (10%)	1 (0%)	47	78
All	All	2531/3028~(84%)	2331 (92%)	195 (8%)	5(0%)	47	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	9	LYS
1	D	221	PRO
1	А	9	LYS
1	В	506	ILE
1	В	584	PRO

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	539/642~(84%)	525~(97%)	14 (3%)	46 77
1	В	537/642~(84%)	524 (98%)	13 (2%)	49 79
1	С	549/642~(86%)	537~(98%)	12 (2%)	52 81
1	D	504/642~(78%)	490 (97%)	14 (3%)	43 76
All	All	2129/2568~(83%)	2076~(98%)	53~(2%)	47 78

analysed, and the total number of residues.

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	112	GLU
1	А	155	ASP
1	А	176	SER
1	А	198	ASP
1	А	220	ILE
1	А	252	SER
1	А	275	TYR
1	А	308	LEU
1	А	336	TRP
1	А	414	VAL
1	А	415	SER
1	А	423	TYR
1	А	464	MET
1	А	538	PHE
1	В	23	MET
1	В	100	TRP
1	В	152	SER
1	В	243	SER
1	В	336	TRP
1	В	384	SER
1	В	388	ASP
1	В	392	ASN
1	В	423	TYR
1	В	465	SER
1	В	522	ARG
1	В	538	PHE
1	В	625	LYS
1	С	21	LYS
1	С	214	THR
1	С	281	SER
1	С	385	SER



Mol	Chain	Res	Type
1	С	392	ASN
1	С	423	TYR
1	С	464	MET
1	С	465	SER
1	С	535	LEU
1	С	538	PHE
1	С	615	SER
1	С	723	ARG
1	D	98	SER
1	D	158	TYR
1	D	184	THR
1	D	251	VAL
1	D	275	TYR
1	D	282	ARG
1	D	294	LEU
1	D	336	TRP
1	D	341	TYR
1	D	425	GLN
1	D	430	ILE
1	D	442	ASP
1	D	520	ASP
1	D	538	PHE

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

Mol	Chain	Res	Type
1	А	392	ASN
1	А	446	ASN
1	С	481	GLN
1	D	446	ASN
1	D	475	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)

14 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	l Type Chain Bes I		Link	Bo	Bond lengths			Bond angles		
	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GOL	D	802	-	$5,\!5,\!5$	0.88	0	$5,\!5,\!5$	1.00	0
2	GOL	В	802	-	$5,\!5,\!5$	0.80	0	$5,\!5,\!5$	0.97	0
4	FMN	С	1604	-	33,33,33	1.08	2(6%)	48,50,50	1.28	9 (18%)
3	BDP	D	801	-	13,13,13	1.41	2 (15%)	18,19,19	1.11	1 (5%)
2	GOL	В	801	-	$5,\!5,\!5$	0.52	0	$5,\!5,\!5$	0.86	0
5	ZG5	С	1601	-	36,37,37	1.74	6 (16%)	$50,\!54,\!54$	3.13	18 (36%)
4	FMN	В	805	-	33,33,33	1.12	2 (6%)	48,50,50	1.35	11 (22%)
3	BDP	В	804	-	13,13,13	1.39	2 (15%)	18,19,19	1.56	3 (16%)
2	GOL	А	801	-	$5,\!5,\!5$	0.86	0	$5,\!5,\!5$	0.93	0
2	GOL	В	803	-	$5,\!5,\!5$	0.65	0	$5,\!5,\!5$	0.83	0
2	GOL	С	1602	-	$5,\!5,\!5$	0.92	0	$5,\!5,\!5$	1.00	0
4	FMN	А	803	-	33,33,33	1.05	2(6%)	48,50,50	1.21	7 (14%)
3	BDP	А	802	-	13,13,13	1.47	2(15%)	18,19,19	2.16	4 (22%)
2	GOL	С	1603	-	5, 5, 5	0.76	0	5, 5, 5	0.93	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	802	-	-	2/4/4/4	-
2	GOL	В	802	-	-	0/4/4/4	-
4	FMN	С	1604	-	-	9/18/18/18	0/3/3/3
3	BDP	D	801	-	-	1/4/24/24	0/1/1/1



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	В	801	-	-	1/4/4/4	-
5	ZG5	С	1601	-	-	7/12/54/54	0/4/5/5
4	FMN	В	805	-	-	8/18/18/18	0/3/3/3
3	BDP	В	804	-	-	0/4/24/24	0/1/1/1
2	GOL	А	801	-	-	2/4/4/4	-
2	GOL	В	803	-	-	2/4/4/4	-
2	GOL	С	1602	-	-	0/4/4/4	-
4	FMN	А	803	-	-	7/18/18/18	0/3/3/3
3	BDP	А	802	-	-	1/4/24/24	0/1/1/1
2	GOL	С	1603	-	-	3/4/4/4	-

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All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	С	1601	ZG5	C11-N10	6.65	1.51	1.37
5	С	1601	ZG5	C11-N12	4.01	1.32	1.29
4	В	805	FMN	C4A-N5	3.75	1.38	1.30
4	С	1604	FMN	C4A-N5	3.73	1.38	1.30
4	А	803	FMN	C4A-N5	3.70	1.37	1.30
3	А	802	BDP	O5-C1	3.13	1.50	1.42
3	D	801	BDP	O5-C1	2.94	1.50	1.42
3	В	804	BDP	O5-C1	2.86	1.50	1.42
5	С	1601	ZG5	C18-S19	2.85	1.80	1.78
4	В	805	FMN	C10-N1	2.78	1.38	1.33
5	С	1601	ZG5	C20-S19	2.74	1.80	1.78
4	С	1604	FMN	C10-N1	2.67	1.38	1.33
4	А	803	FMN	C10-N1	2.61	1.38	1.33
3	А	802	BDP	O5-C5	2.60	1.47	1.43
5	С	1601	ZG5	C25-C20	-2.59	1.36	1.40
3	В	804	BDP	O5-C5	2.36	1.47	1.43
5	С	1601	ZG5	O05-C04	-2.23	1.39	1.43
3	D	801	BDP	O5-C5	2.11	1.47	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	С	1601	ZG5	N10-C11-N12	-13.13	108.31	118.30
5	С	1601	ZG5	C13-N12-C11	10.78	137.04	123.03
5	С	1601	ZG5	C20-C25-C11	5.09	129.94	121.95
3	А	802	BDP	C1-O5-C5	4.83	119.32	112.22
5	С	1601	ZG5	C20-S19-C18	4.37	110.61	99.13



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	С	1601	ZG5	C18-C13-N12	4.11	128.25	123.37
3	А	802	BDP	O5-C5-C4	4.03	116.78	109.57
5	С	1601	ZG5	C26-C27-N07	4.00	118.24	110.59
3	А	802	BDP	O5-C1-C2	3.77	117.02	110.28
5	С	1601	ZG5	C25-C11-N12	-3.48	122.91	125.88
3	А	802	BDP	O2-C2-C3	-3.40	102.49	110.35
3	В	804	BDP	O5-C1-C2	3.34	116.25	110.28
5	С	1601	ZG5	C23-C24-C25	3.30	126.06	119.81
5	С	1601	ZG5	C26-N10-C09	-3.28	106.31	112.62
5	С	1601	ZG5	O05-C06-C28	3.07	114.90	110.15
4	А	803	FMN	C4-N3-C2	-3.06	120.00	125.64
5	С	1601	ZG5	C22-C23-C24	-3.03	115.57	120.19
4	С	1604	FMN	C4-N3-C2	-3.03	120.05	125.64
4	В	805	FMN	C4-N3-C2	-3.00	120.10	125.64
5	С	1601	ZG5	O05-C04-C02	2.87	113.59	105.88
3	В	804	BDP	O2-C2-C3	-2.77	103.94	110.35
3	D	801	BDP	O2-C2-C3	-2.76	103.97	110.35
4	А	803	FMN	C4A-C10-N10	2.71	120.45	116.48
4	С	1604	FMN	C5'-C4'-C3'	-2.67	107.05	112.20
5	С	1601	ZG5	O33-C32-C30	-2.64	104.23	110.35
4	В	805	FMN	C4A-C10-N1	-2.64	118.60	124.73
4	А	803	FMN	C4A-C4-N3	2.63	119.86	113.19
4	С	1604	FMN	C4A-C4-N3	2.61	119.82	113.19
4	С	1604	FMN	C4A-C10-N10	2.59	120.27	116.48
4	В	805	FMN	C5A-C9A-N10	2.57	120.61	117.95
3	В	804	BDP	C1-C2-C3	2.56	115.62	110.31
4	В	805	FMN	C4-C4A-C10	2.55	121.07	116.79
4	С	1604	FMN	C4A-C10-N1	-2.49	118.94	124.73
4	С	1604	FMN	O4-C4-C4A	-2.45	120.09	126.60
4	В	805	FMN	C4A-C4-N3	2.45	119.41	113.19
4	A	803	FMN	O4-C4-C4A	-2.44	120.13	126.60
4	В	805	FMN	O4-C4-C4A	-2.43	120.16	126.60
4	A	803	FMN	C4A-C10-N1	-2.38	119.21	124.73
5	С	1601	ZG5	O31-C30-C32	-2.34	104.94	110.35
4	В	805	FMN	C4A-C10-N10	2.33	119.89	116.48
4	В	805	FMN	C1'-C2'-C3'	2.30	116.20	109.79
5	С	1601	ZG5	C14-C13-C18	-2.28	115.77	119.01
5	С	1601	ZG5	C15-C14-C13	2.27	123.25	118.98
4	A	803	FMN	C10-C4A-N5	-2.27	120.04	124.86
4	С	1604	FMN	C10-C4A-N5	-2.25	120.08	124.86
4	В	805	FMN	$C10-C\overline{4A-N5}$	-2.12	120.35	124.86
5	С	1601	ZG5	C08-N07-C06	-2.11	110.16	115.09



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	1604	FMN	C4-C4A-C10	2.11	120.33	116.79
4	В	805	FMN	C9A-C5A-N5	-2.09	120.17	122.43
4	А	803	FMN	C4-C4A-C10	2.04	120.22	116.79
5	С	1601	ZG5	C24-C25-C11	-2.02	113.54	118.96
4	В	805	FMN	O4'-C4'-C3'	2.02	114.01	109.10
4	С	1604	FMN	C5A-C9A-N10	2.01	120.03	117.95

There are no chirality outliers.

Mol	Chain	Res	Type	Atoms
2	А	801	GOL	C1-C2-C3-O3
2	В	803	GOL	C1-C2-C3-O3
2	В	803	GOL	O2-C2-C3-O3
2	D	802	GOL	C1-C2-C3-O3
4	А	803	FMN	C1'-C2'-C3'-O3'
4	А	803	FMN	C1'-C2'-C3'-C4'
4	А	803	FMN	O2'-C2'-C3'-O3'
4	А	803	FMN	O2'-C2'-C3'-C4'
4	А	803	FMN	C5'-O5'-P-O1P
4	А	803	FMN	C5'-O5'-P-O2P
4	В	805	FMN	C1'-C2'-C3'-O3'
4	В	805	FMN	C1'-C2'-C3'-C4'
4	В	805	FMN	O2'-C2'-C3'-O3'
4	В	805	FMN	O2'-C2'-C3'-C4'
4	В	805	FMN	C2'-C3'-C4'-O4'
4	В	805	FMN	C2'-C3'-C4'-C5'
4	В	805	FMN	O3'-C3'-C4'-O4'
4	В	805	FMN	O3'-C3'-C4'-C5'
4	С	1604	FMN	C1'-C2'-C3'-O3'
4	С	1604	FMN	C1'-C2'-C3'-C4'
4	С	1604	FMN	O2'-C2'-C3'-O3'
4	С	1604	FMN	O2'-C2'-C3'-C4'
4	С	1604	FMN	C3'-C4'-C5'-O5'
4	С	1604	FMN	O4'-C4'-C5'-O5'
4	С	1604	FMN	C5'-O5'-P-O1P
4	С	1604	FMN	C5'-O5'-P-O2P
4	C	1604	FMN	C5'-O5'-P-O3P
5	С	1601	ZG5	C28-C06-N07-C08
5	С	1601	ZG5	C28-C06-N07-C27
5	С	1601	ZG5	O05-C06-N07-C27
5	С	1601	ZG5	N12-C11-N10-C09

All (43) torsion outliers are listed below:



Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	801	GOL	C1-C2-C3-O3
2	С	1603	GOL	C1-C2-C3-O3
5	С	1601	ZG5	N12-C11-N10-C26
2	А	801	GOL	O2-C2-C3-O3
2	D	802	GOL	O2-C2-C3-O3
3	А	802	BDP	O5-C5-C6-O6A
5	С	1601	ZG5	O01-C02-C04-O05
5	С	1601	ZG5	O05-C06-N07-C08
2	С	1603	GOL	O2-C2-C3-O3
4	А	803	FMN	C5'-O5'-P-O3P
2	С	1603	GOL	O1-C1-C2-C3
3	D	801	BDP	O5-C5-C6-O6B

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There are no ring outliers.

11 monomers are	involved	in 20	short	contacts:
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	1604	FMN	2	0
3	D	801	BDP	1	0
5	С	1601	ZG5	1	0
4	В	805	FMN	3	0
3	В	804	BDP	3	0
2	А	801	GOL	1	0
2	В	803	GOL	1	0
2	С	1602	GOL	2	0
4	А	803	FMN	1	0
3	А	802	BDP	2	0
2	С	1603	GOL	3	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 similar 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	639/757~(84%)	0.12	12 (1%) 66 65	30, 62, 92, 135	0
1	В	644/757~(85%)	0.15	17 (2%) 56 52	30, 65, 92, 119	0
1	С	659/757~(87%)	0.12	21 (3%) 47 43	41, 60, 94, 127	1 (0%)
1	D	623/757~(82%)	0.35	28 (4%) 33 29	30, 77, 110, 137	0
All	All	2565/3028~(84%)	0.19	78 (3%) 50 45	30, 66, 99, 137	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	179	VAL	4.3
1	D	636	PHE	3.9
1	D	149	VAL	3.8
1	D	195	THR	3.5
1	D	272	GLY	3.4
1	D	192	LEU	3.4
1	D	220	ILE	3.3
1	D	218	LEU	3.2
1	А	223	VAL	3.0
1	А	65	PRO	3.0
1	С	207	THR	3.0
1	С	191	LYS	3.0
1	В	383	GLY	3.0
1	D	180	GLU	3.0
1	D	194	TYR	3.0
1	D	237	ALA	2.9
1	В	248	VAL	2.9
1	В	636	PHE	2.8
1	D	168	PRO	2.8
1	D	214	THR	2.8
1	С	719	PHE	2.8



Mol	Chain	Res	Type	RSRZ
1	С	176	SER	2.8
1	С	440	GLY	2.8
1	А	204	VAL	2.7
1	В	635	THR	2.7
1	С	726	ASN	2.7
1	D	65	PRO	2.6
1	D	224	HIS	2.6
1	В	612	VAL	2.6
1	В	187	ALA	2.6
1	В	183	LEU	2.6
1	В	247	ALA	2.6
1	D	246	GLU	2.6
1	D	638	GLU	2.6
1	D	236	THR	2.5
1	В	568	VAL	2.5
1	В	192	LEU	2.5
1	А	247	ALA	2.4
1	С	722	ILE	2.4
1	А	196	VAL	2.4
1	D	190	GLN	2.4
1	А	67	ALA	2.4
1	В	641	SER	2.4
1	D	178	GLU	2.4
1	С	192	LEU	2.4
1	А	209	THR	2.3
1	D	635	THR	2.3
1	С	612	VAL	2.3
1	С	209	THR	2.3
1	А	242	VAL	2.3
1	С	173	ALA	2.3
1	С	218	LEU	2.3
1	С	203	GLU	2.3
1	В	477	SER	2.2
1	D	176	SER	2.2
1	С	220	ILE	2.2
1	А	218	LEU	2.2
1	А	622	GLY	2.2
1	В	211	ALA	2.2
1	C	241	LEU	2.2
1	В	642	LEU	2.2
1	С	208	GLU	2.2
1	В	218	LEU	2.2



Mol	Chain	Res	Type	RSRZ
1	А	588	LEU	2.2
1	D	171	LYS	2.2
1	В	633	VAL	2.1
1	D	196	VAL	2.1
1	А	419	ILE	2.1
1	С	174	ASP	2.1
1	С	211	ALA	2.1
1	С	593	LYS	2.1
1	D	609	VAL	2.1
1	В	112	GLU	2.0
1	D	256	GLY	2.0
1	D	191	LYS	2.0
1	С	623	GLU	2.0
1	D	439	TYR	2.0
1	С	728	MET	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	\mathbf{Res}	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BDP	В	804	13/13	0.77	0.33	$55,\!67,\!95,\!98$	22
2	GOL	В	801	6/6	0.80	0.40	76,103,117,120	0
3	BDP	D	801	13/13	0.80	0.24	83,100,127,142	22
2	GOL	А	801	6/6	0.84	0.36	64,91,118,118	0
2	GOL	В	803	6/6	0.84	0.34	80,114,125,128	0
4	FMN	С	1604	31/31	0.85	0.23	78,91,104,123	0
2	GOL	D	802	6/6	0.86	0.27	67,97,115,115	0
4	FMN	А	803	31/31	0.87	0.20	77,87,96,111	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	С	1602	6/6	0.88	0.32	$68,\!105,\!116,\!142$	0
4	FMN	В	805	31/31	0.90	0.20	63,78,93,102	0
3	BDP	А	802	13/13	0.90	0.21	53,67,86,101	22
2	GOL	С	1603	6/6	0.91	0.33	55,82,102,102	0
5	ZG5	С	1601	33/33	0.91	0.26	43,67,97,107	0
2	GOL	В	802	6/6	0.96	0.27	55,83,98,101	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.

