

Full wwPDB X-ray Structure Validation Report (i)

May 22, 2020 – 10:33 pm BST

Title : Crystal structure of plasmepsin IV from P. falciparum in complex	with pep-
statin A	
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Deposited on : 2002-05-16	
${\rm Resolution} : 2.80 {\rm \AA}({\rm reported})$	

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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain					
1	А	328	27%	61%	12% •			
1	В	328	33%	53%	13% •			
2	С	6	17%	50%	33%			
2	D	6	50%	17%	33%			



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5342 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 plasmepsin IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	328	Total 2609	C 1686	N 397	O 515	S 11	0	0	0
1	В	328	Total 2609	C 1686	N 397	O 515	S 11	0	0	0

• Molecule 2 is a protein called Pepstatin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	С	6	Total C N O 48 34 5 9	0	0	0
2	D	6	Total C N O 48 34 5 9	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	18	Total O 18 18	0	0
3	В	10	Total O 10 10	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. Residues are colorcoded 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. 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.

Note EDS was not executed.

• Molecule 1: plasmepsin IV



• Molecule 1: plasmepsin IV





734 V35 V35 V35 V35 V35 V35 V35 V35 V35

• Molecule 2: Pepstatin

Chain C:	17%	50%		33%			
71 V2 V3 85 85 76							
• Molecule 2: Pepstatin							
Chain D:	509	%	17%	33%			



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	101.93Å 101.93Å 123.39Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 - 2.80	Depositor
% Data completeness	(Not available) (10.00-2.80)	Depositor
(in resolution range)	(100 available) (10.00 2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.220 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5342	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP



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: STA, IVA

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	0.45	0/2677	0.73	0/3637	
1	В	0.45	0/2677	0.75	2/3637~(0.1%)	
2	С	0.84	0/17	2.54	1/21~(4.8%)	
2	D	0.84	0/17	2.66	1/21~(4.8%)	
All	All	0.45	0/5388	0.76	4/7316~(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	С	0	2
2	D	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	350	VAL	CG1-CB-CG2	-8.53	97.25	110.90
2	С	2	VAL	CG1-CB-CG2	-8.15	97.85	110.90
1	В	242	LEU	N-CA-C	6.27	127.93	111.00
1	В	198	ASP	N-CA-C	-5.30	96.70	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	С	4	STA	Mainchain,Peptide
2	D	352	STA	Mainchain,Peptide

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	2609	0	2501	391	8
1	В	2609	0	2501	261	7
2	С	48	0	60	11	0
2	D	48	0	60	5	0
3	А	18	0	0	5	0
3	В	10	0	0	1	0
All	All	5342	0	5122	641	8

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 61.

All (641) 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:277:LEU:HD22	1:B:280:ILE:HD13	1.33	1.09
1:B:310:PHE:HB2	1:B:325:ALA:HB2	1.39	1.04
1:A:74:GLU:HG2	1:A:83:ARG:HG2	1.38	1.04
1:B:221:THR:HB	1:B:300:ILE:HB	1.39	1.02
1:A:307:ARG:HB2	1:A:307:ARG:HH11	1.26	1.00
1:A:251:ASN:HD22	1:A:252:ASP:H	1.08	0.99
1:B:247:THR:HG22	1:B:248:THR:H	1.29	0.97
1:A:251:ASN:ND2	1:A:252:ASP:H	1.63	0.95
1:A:307:ARG:HB2	1:A:307:ARG:NH1	1.83	0.94
1:B:178:TYR:HA	1:B:325:ALA:HA	1.50	0.93
1:A:281:ASP:OD2	1:B:281:ASP:HB2	1.66	0.93
1:A:5:SER:HB3	1:A:169:THR:HG22	1.49	0.92
1:A:269:GLU:H	1:A:308:LYS:HZ1	1.17	0.92
1:A:275:ASP:H	1:A:285:CYS:HB2	1.33	0.92
1:A:244:LEU:HD21	1:A:288:TYR:HD2	1.33	0.91
1:B:198:ASP:HB3	1:B:260:HIS:HB2	1.52	0.91



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:13:ASN:HB2	1:A:307:ARG:HH21	1.36	0.90
1:A:236:VAL:HG12	1:A:245:TYR:HB3	1.51	0.90
1:B:294:ILE:H	1:B:294:ILE:HD12	1.33	0.89
1:A:314:ASP:OD2	1:A:317:LYS:HD2	1.72	0.88
1:A:144:LYS:HG2	1:A:152:ALA:HB2	1.52	0.88
1:B:241:PHE:O	1:B:243:PRO:HD3	1.74	0.87
1:B:19:GLU:CD	1:B:19:GLU:H	1.79	0.86
1:A:27:GLN:HE22	1:A:59:ASP:H	1.23	0.85
1:B:138:PRO:HB2	1:B:141:VAL:HG23	1.58	0.85
1:A:221:THR:HB	1:A:300:ILE:HB	1.59	0.85
1:B:303:ASP:O	1:B:307:ARG:HG2	1.76	0.84
1:A:114:ILE:H	1:A:114:ILE:HD12	1.40	0.84
1:A:251:ASN:HD22	1:A:252:ASP:N	1.75	0.83
1:B:247:THR:HG22	1:B:248:THR:N	1.94	0.82
1:A:277:LEU:HD21	1:A:286:MET:HG2	1.63	0.81
1:A:13:ASN:HB3	1:A:161:HIS:HA	1.61	0.81
1:A:79:SER:HB3	1:A:114:ILE:HG12	1.63	0.81
1:A:303:ASP:HB3	1:A:307:ARG:HH12	1.45	0.80
1:A:244:LEU:HD12	1:A:286:MET:HE3	1.63	0.80
1:A:244:LEU:HD21	1:A:288:TYR:HA	1.64	0.80
1:A:293:ASP:HB2	1:B:50:ILE:HD11	1.63	0.80
1:A:326:LYS:O	1:A:328:LEU:N	2.13	0.79
1:B:276:PRO:HA	1:B:285:CYS:SG	2.22	0.79
1:A:236:VAL:CG1	1:A:245:TYR:HB3	2.13	0.79
1:A:18:GLY:HA3	1:A:33:PHE:HE1	1.47	0.79
1:A:199:ILE:HD13	1:A:209:ALA:HB3	1.63	0.79
1:B:263:ASN:O	1:B:264:ASN:HB2	1.83	0.79
1:A:17:TYR:CE2	1:A:119:GLU:HB2	2.19	0.78
1:A:293:ASP:HB2	1:B:50:ILE:CD1	2.14	0.78
1:A:185:GLU:O	1:A:319:SER:HB2	1.84	0.78
1:B:258:GLU:HB3	1:B:267:THR:HG22	1.64	0.77
1:B:142:GLU:HG3	1:B:146:GLN:HE21	1.48	0.77
1:B:268:LEU:HD23	1:B:308:LYS:HD2	1.66	0.77
1:A:277:LEU:HD13	1:A:285:CYS:HA	1.65	0.77
1:A:12:ALA:O	1:A:14:LEU:HD12	1.84	0.77
1:A:275:ASP:N	1:A:285:CYS:HB2	2.00	0.77
1:A:242:LEU:HD12	1:A:243:PRO:HA	1.67	0.77
1:B:236:VAL:HB	1:B:287:LEU:HD22	1.65	0.77
1:B:239:VAL:HG13	1:B:240:PRO:HD2	1.67	0.77
1:B:251:ASN:HB3	1:B:254:LEU:HD11	1.67	0.75
1:A:209:ALA:HA	1:A:297:ASN:HD21	1.52	0.75



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:209:ALA:HA	1:A:297:ASN:ND2	2.02	0.74
1:A:284:LEU:HD22	1:B:280:ILE:HG23	1.67	0.74
1:A:281:ASP:HB2	1:A:284:LEU:HD13	1.69	0.74
1:A:198:ASP:OD1	1:A:207:GLN:HA	1.86	0.74
1:A:242:LEU:HD12	1:A:243:PRO:CA	2.17	0.74
1:A:290:LEU:HD23	1:A:291:PRO:HD2	1.68	0.73
1:A:293:ASP:HB2	1:B:50:ILE:CG1	2.17	0.73
1:B:12:ALA:HB3	1:B:14:LEU:HD11	1.69	0.73
1:B:308:LYS:HD3	1:B:309:TYR:CE2	2.23	0.73
1:B:200:HIS:HB2	1:B:258:GLU:HG3	1.70	0.73
1:B:244:LEU:HG	1:B:286:MET:HE1	1.69	0.73
1:A:244:LEU:CD2	1:A:288:TYR:HA	2.19	0.73
1:A:221:THR:O	1:A:299:PHE:HA	1.89	0.73
1:A:178:TYR:HE2	1:A:182:LEU:HB2	1.54	0.72
1:B:73:VAL:HG11	1:B:86:PHE:CE2	2.24	0.72
1:A:270:PRO:HA	1:A:273:TYR:CZ	2.25	0.71
1:A:5:SER:CB	1:A:169:THR:HG22	2.21	0.71
1:A:13:ASN:HD22	1:A:307:ARG:CZ	2.04	0.71
1:B:91:ILE:HD13	1:B:100:TYR:HB3	1.72	0.71
1:B:239:VAL:HG12	1:B:243:PRO:HG2	1.71	0.70
1:B:277:LEU:HB2	1:B:284:LEU:O	1.91	0.70
1:A:219:THR:HG22	1:A:220:ILE:O	1.92	0.70
1:A:96:LEU:HD11	1:A:149:ILE:HD13	1.73	0.70
1:A:40:LEU:HD12	1:A:41:TRP:N	2.07	0.70
1:B:244:LEU:HD13	1:B:244:LEU:H	1.56	0.70
1:A:5:SER:HA	1:A:169:THR:HA	1.72	0.70
1:A:178:TYR:CE2	1:A:182:LEU:HB2	2.26	0.69
1:A:293:ASP:HB2	1:B:50:ILE:HG12	1.74	0.69
1:B:246:VAL:HG12	1:B:247:THR:N	2.07	0.69
1:A:246:VAL:HB	1:A:286:MET:SD	2.32	0.69
1:B:163:LYS:HG3	1:B:164:HIS:NE2	2.08	0.68
1:B:155:THR:N	1:B:169:THR:O	2.22	0.68
1:A:220:ILE:HB	1:A:289:ILE:HD13	1.76	0.68
1:A:27:GLN:HE22	1:A:59:ASP:N	1.91	0.68
1:B:103:ILE:N	1:B:103:ILE:HD12	2.09	0.68
1:B:144:LYS:HA	1:B:149:ILE:HG22	1.76	0.68
1:B:222:ALA:HB3	1:B:227:LEU:HD13	1.76	0.68
1:B:44:SER:HB2	1:B:104:GLU:OE2	1.94	0.68
1:B:227:LEU:HD11	1:B:289:ILE:HG22	1.76	0.67
1:B:40:LEU:HD12	1:B:41:TRP:N	2.08	0.67
1:A:294:ILE:HG23	2:C:6:STA:HD13	1.74	0.67



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:165:VAL:O	1:B:165:VAL:HG13	1.93	0.67
1:B:247:THR:CG2	1:B:248:THR:H	2.05	0.67
1:B:221:THR:CG2	1:B:292:VAL:HB	2.25	0.67
1:A:269:GLU:H	1:A:308:LYS:NZ	1.91	0.67
1:A:160:VAL:HG22	1:A:307:ARG:HG3	1.78	0.66
1:B:254:LEU:HD12	1:B:254:LEU:N	2.10	0.66
1:B:227:LEU:CD2	1:B:291:PRO:HB3	2.25	0.66
1:B:178:TYR:CA	1:B:325:ALA:HA	2.26	0.66
1:A:178:TYR:C	1:A:326:LYS:HD2	2.15	0.66
1:A:307:ARG:CB	1:A:307:ARG:HH11	2.06	0.66
1:A:244:LEU:HD21	1:A:288:TYR:CD2	2.25	0.65
1:B:59:ASP:OD2	1:B:62:ALA:HB2	1.97	0.65
1:A:42:VAL:HG11	1:A:58:TYR:HB2	1.78	0.65
1:A:73:VAL:HG21	1:A:103:ILE:HD13	1.79	0.65
1:B:221:THR:HB	1:B:300:ILE:CB	2.22	0.65
1:B:275:ASP:HB2	1:B:286:MET:HB2	1.79	0.65
1:A:153:LEU:HB2	1:A:313:PHE:O	1.96	0.65
1:A:27:GLN:NE2	1:A:59:ASP:H	1.94	0.65
1:A:124:LEU:HD23	1:A:125:GLY:O	1.95	0.64
1:A:200:HIS:HB2	1:A:204:TYR:O	1.97	0.64
1:A:222:ALA:HB3	1:A:227:LEU:CD1	2.27	0.64
1:A:268:LEU:HA	1:A:308:LYS:HE3	1.77	0.64
1:A:67:GLU:HB2	1:A:88:LYS:NZ	2.12	0.64
1:B:200:HIS:CB	1:B:258:GLU:HG3	2.27	0.64
1:A:55:LYS:HB2	1:A:121:ASP:OD1	1.97	0.64
1:A:24:THR:C	1:A:26:LYS:H	2.02	0.64
1:A:2:GLU:O	1:A:3:ASN:ND2	2.31	0.63
1:A:260:HIS:HB3	1:A:265:LYS:CB	2.29	0.63
1:A:268:LEU:HD12	1:A:308:LYS:HE2	1.79	0.63
1:B:111:LEU:HG	1:B:115:TYR:HB2	1.79	0.63
1:A:13:ASN:HD22	1:A:307:ARG:NH2	1.96	0.63
1:A:239:VAL:HG22	1:A:246:VAL:HG12	1.79	0.63
1:A:12:ALA:O	1:A:13:ASN:OD1	2.17	0.63
1:B:3:ASN:HB3	1:B:170:ILE:O	1.98	0.63
1:A:234:MET:HB3	1:A:236:VAL:HG23	1.80	0.63
1:A:222:ALA:HB3	1:A:227:LEU:HD13	1.81	0.62
1:A:281:ASP:HB2	1:A:284:LEU:CD1	2.28	0.62
1:A:73:VAL:HG11	1:A:86:PHE:CE2	2.33	0.62
1:B:163:LYS:HG3	1:B:164:HIS:CE1	2.34	0.62
1:B:218:SER:HA	1:B:303:ASP:OD2	1.99	0.62
1:A:18:GLY:HA3	1:A:33:PHE:CE1	2.31	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:305:PHE:HD2	1:B:305:PHE:O	1.81	0.62
1:A:144:LYS:CG	1:A:152:ALA:HB2	2.27	0.62
1:A:260:HIS:N	1:A:260:HIS:CD2	2.68	0.62
2:C:2:VAL:HG11	2:C:4:STA:HD23	1.82	0.62
1:A:174:GLU:HB3	1:A:177:PHE:CE2	2.34	0.61
1:A:251:ASN:ND2	1:A:252:ASP:N	2.39	0.61
2:C:2:VAL:HG12	2:C:4:STA:HB2	1.83	0.61
1:A:210:ASN:HD22	1:A:298:THR:HG23	1.66	0.61
1:A:278:SER:HA	1:A:282:PRO:HA	1.82	0.61
1:A:238:LYS:HB2	1:A:245:TYR:CE2	2.36	0.61
1:A:159:PRO:HB3	1:A:164:HIS:ND1	2.16	0.61
1:A:192:TYR:O	1:A:194:GLN:HG2	2.01	0.61
1:A:73:VAL:HG21	1:A:103:ILE:CD1	2.30	0.61
1:A:269:GLU:N	1:A:308:LYS:HZ1	1.95	0.61
1:B:14:LEU:HD23	1:B:288:TYR:CE2	2.36	0.61
1:A:284:LEU:N	1:A:284:LEU:HD12	2.16	0.60
1:A:304:PRO:HD2	3:A:366:HOH:O	2.01	0.60
1:B:238:LYS:HD2	1:B:242:LEU:H	1.66	0.60
1:B:204:TYR:CE2	1:B:229:LYS:HB3	2.36	0.60
1:B:281:ASP:OD2	1:B:283:ALA:HB3	2.02	0.60
1:A:177:PHE:O	1:A:326:LYS:HG2	2.02	0.60
1:A:234:MET:HB3	1:A:236:VAL:CG2	2.32	0.60
1:A:241:PHE:N	1:A:241:PHE:CD2	2.70	0.60
1:A:256:THR:HG23	1:A:268:LEU:O	2.02	0.60
1:A:277:LEU:HB2	1:A:284:LEU:O	2.02	0.60
1:B:242:LEU:O	1:B:243:PRO:C	2.40	0.60
1:A:218:SER:HA	1:A:303:ASP:OD2	2.02	0.60
1:B:178:TYR:O	1:B:326:LYS:HE2	2.01	0.59
1:B:187:LEU:HB3	1:B:189:HIS:O	2.02	0.59
1:A:163:LYS:HG2	1:A:164:HIS:CG	2.38	0.59
1:B:159:PRO:O	1:B:160:VAL:HG23	2.03	0.59
1:B:248:THR:HG23	1:B:250:ASP:OD1	2.03	0.59
1:B:237:ILE:N	1:B:246:VAL:O	2.35	0.59
1:B:210:ASN:O	1:B:298:THR:HA	2.03	0.59
1:A:309:TYR:HA	1:A:325:ALA:H	1.67	0.59
1:A:27:GLN:HE22	1:A:58:TYR:HA	1.66	0.59
1:A:188:ASN:C	1:A:189:HIS:ND1	2.56	0.59
1:A:221:THR:CG2	1:A:292:VAL:HB	2.32	0.59
1:B:239:VAL:CG1	1:B:243:PRO:HG2	2.31	0.59
1:A:293:ASP:CB	1:B:50:ILE:HD11	2.31	0.59
1:B:159:PRO:HB3	1:B:164:HIS:ND1	$2.\overline{18}$	0.59



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:B:17:TYR:HB3	1:B:32:ILE:HD13	1.84	0.59
1:B:84:GLY:HA3	1:B:104:GLU:O	2.02	0.59
1:A:20:GLY:HA3	1:A:31:PHE:CD2	2.38	0.58
1:A:178:TYR:HD2	1:A:323:ALA:HB1	1.68	0.58
1:B:3:ASN:O	1:B:4:ASP:HB2	2.03	0.58
1:A:14:LEU:O	1:A:15:MET:HB3	2.02	0.58
1:A:303:ASP:O	1:A:307:ARG:N	2.36	0.58
1:B:238:LYS:NZ	1:B:241:PHE:HA	2.19	0.58
1:A:187:LEU:O	1:A:189:HIS:N	2.33	0.58
1:B:40:LEU:HG	1:B:102:PHE:CB	2.34	0.58
1:B:199:ILE:HD12	1:B:209:ALA:HB3	1.84	0.58
1:A:19:GLU:N	1:A:19:GLU:OE1	2.36	0.58
1:A:36:GLY:HA3	2:C:4:STA:HM2	1.84	0.58
1:B:227:LEU:HD23	1:B:291:PRO:HB3	1.85	0.58
1:A:220:ILE:HG22	1:A:221:THR:N	2.18	0.58
1:A:89:ASP:OD1	1:A:90:VAL:N	2.34	0.57
1:A:174:GLU:OE1	1:A:176:ASP:HB2	2.04	0.57
1:A:189:HIS:HB2	1:A:194:GLN:OE1	2.03	0.57
1:A:174:GLU:CD	1:A:176:ASP:H	2.08	0.57
1:A:27:GLN:NE2	1:A:58:TYR:HA	2.18	0.57
1:B:29:PHE:CD2	1:B:42:VAL:HG21	2.39	0.57
1:A:188:ASN:OD1	1:A:195:ILE:HA	2.05	0.57
1:A:187:LEU:HD23	1:A:190:ASP:OD1	2.03	0.57
1:A:83:ARG:NH1	1:A:107:ASP:OD1	2.38	0.57
1:A:232:ARG:HH11	1:A:232:ARG:HA	1.70	0.57
1:A:10:ASP:OD2	1:A:16:PHE:CE2	2.58	0.57
1:B:272:PHE:CD2	1:B:308:LYS:HB2	2.39	0.56
1:A:247:THR:HG22	1:A:248:THR:H	1.70	0.56
1:A:13:ASN:CB	1:A:307:ARG:HH21	2.14	0.56
1:B:163:LYS:HG3	1:B:164:HIS:CD2	2.40	0.56
1:B:4:ASP:OD2	1:B:94:GLY:HA3	2.04	0.56
2:D:350:VAL:HG11	2:D:352:STA:HD23	1.87	0.56
1:A:155:THR:HB	1:A:169:THR:OG1	2.05	0.56
1:B:142:GLU:HG3	1:B:146:GLN:NE2	2.18	0.56
1:A:176:ASP:O	1:A:326:LYS:HD3	2.05	0.56
1:A:295:ASP:O	1:A:296:ASP:HB2	2.05	0.56
1:B:233:ASP:HB2	1:B:234:MET:HE2	1.87	0.56
1:B:246:VAL:CG1	1:B:247:THR:N	2.69	0.56
1:B:254:LEU:HD22	1:B:274:MET:HE1	1.86	0.56
1:B:4:ASP:OD1	1:B:95:ASP:OD2	2.23	$0.\overline{56}$
1:B:244:LEU:HD13	1:B:244:LEU:N	2.21	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:210:ASN:ND2	1:A:298:THR:HG23	2.21	0.56
1:A:35:THR:HG23	1:A:215:SER:OG	2.06	0.56
1:B:294:ILE:HG12	1:B:298:THR:O	2.05	0.56
1:A:275:ASP:CB	1:A:276:PRO:HA	2.36	0.56
1:A:279:ASP:HB3	1:B:237:ILE:HD13	1.87	0.56
1:A:197:LEU:HD23	1:A:261:SER:HB3	1.89	0.55
1:B:219:THR:HG22	1:B:288:TYR:HB3	1.87	0.55
1:A:74:GLU:HG2	1:A:83:ARG:CG	2.24	0.55
1:B:12:ALA:O	1:B:13:ASN:HB2	2.06	0.55
1:B:249:CYS:HB2	1:B:283:ALA:O	2.06	0.55
1:A:14:LEU:HD22	2:C:1:IVA:HG13	1.88	0.55
1:B:138:PRO:HB2	1:B:141:VAL:CG2	2.36	0.55
1:B:29:PHE:CE2	1:B:42:VAL:HG21	2.42	0.55
1:A:312:VAL:O	1:A:321:GLY:N	2.37	0.55
1:A:224:THR:HG22	1:A:228:ASN:HD21	1.72	0.55
1:B:206:MET:HG2	1:B:209:ALA:HB2	1.88	0.55
1:A:79:SER:OG	2:C:2:VAL:HG13	2.07	0.55
1:B:12:ALA:HB3	1:B:14:LEU:CD1	2.35	0.54
1:A:178:TYR:CE2	1:A:182:LEU:HD13	2.42	0.54
1:A:79:SER:O	1:A:114:ILE:HD13	2.07	0.54
1:B:242:LEU:HD23	1:B:242:LEU:C	2.26	0.54
1:A:50:ILE:C	1:A:52:CYS:H	2.10	0.54
1:A:21:GLN:HB2	1:A:92:SER:HB2	1.90	0.54
1:A:221:THR:HG21	1:A:292:VAL:HB	1.88	0.54
1:A:284:LEU:HD22	1:B:280:ILE:CG2	2.36	0.54
1:B:40:LEU:HG	1:B:102:PHE:HB2	1.89	0.54
1:B:83:ARG:NH1	1:B:107:ASP:OD2	2.40	0.54
1:A:275:ASP:HA	1:A:285:CYS:HB2	1.89	0.54
1:B:236:VAL:HG23	1:B:246:VAL:O	2.07	0.54
1:B:253:ASP:CG	1:B:253:ASP:O	2.45	0.54
1:A:280:ILE:HA	1:B:284:LEU:HD12	1.90	0.54
1:A:17:TYR:HE2	1:A:119:GLU:HB2	1.70	0.54
1:B:160:VAL:O	1:B:162:ASP:N	2.40	0.54
1:A:182:LEU:HD12	1:A:323:ALA:HB2	1.89	0.54
1:B:256:THR:HG22	1:B:267:THR:HB	1.90	0.54
1:A:160:VAL:HG23	1:A:163:LYS:HZ1	1.72	0.54
1:A:16:PHE:N	1:A:16:PHE:CD1	2.75	0.54
1:A:74:GLU:OE1	1:A:83:ARG:HD2	2.08	0.54
1:A:13:ASN:OD1	1:A:14:LEU:HD12	2.09	0.53
1:A:219:THR:HG21	1:A:290:LEU:H	1.73	0.53
1:A:162:ASP:O	1:A:163:LYS:HB3	2.09	0.53



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:24:THR:HG23	1:B:65:SER:OG	2.08	0.53
1:A:13:ASN:O	1:A:307:ARG:NH2	2.41	0.53
1:A:113:PRO:HG3	1:B:78:GLY:O	2.07	0.53
1:A:303:ASP:HB2	1:A:304:PRO:HD3	1.90	0.53
1:B:7:GLU:OE1	1:B:165:VAL:HG11	2.09	0.53
1:A:131:LEU:HB2	1:A:191:LEU:HD13	1.90	0.53
1:A:40:LEU:HG	1:A:102:PHE:HB2	1.91	0.53
1:A:65:SER:HB2	1:A:90:VAL:HG23	1.91	0.53
1:A:242:LEU:HD12	1:A:243:PRO:CB	2.39	0.53
1:A:245:TYR:HB2	1:A:287:LEU:HD23	1.89	0.53
1:B:11:VAL:HG21	1:B:17:TYR:OH	2.08	0.53
1:B:227:LEU:HD22	1:B:291:PRO:HB3	1.91	0.53
1:A:260:HIS:HB3	1:A:265:LYS:HA	1.89	0.53
1:A:275:ASP:CA	1:A:285:CYS:HB2	2.39	0.53
1:B:244:LEU:C	1:B:245:TYR:CD1	2.82	0.53
1:A:163:LYS:HG2	1:A:164:HIS:N	2.24	0.52
1:A:177:PHE:C	1:A:326:LYS:HG2	2.30	0.52
1:B:67:GLU:HB3	1:B:88:LYS:HB2	1.90	0.52
1:B:241:PHE:C	1:B:243:PRO:HD3	2.29	0.52
1:A:197:LEU:CD2	1:A:261:SER:HB3	2.40	0.52
1:A:277:LEU:HD13	1:A:286:MET:H	1.74	0.52
1:A:114:ILE:H	1:A:114:ILE:CD1	2.13	0.52
1:A:226:PHE:O	1:A:226:PHE:CD1	2.63	0.52
1:A:236:VAL:HG11	1:A:287:LEU:HD22	1.92	0.52
1:A:83:ARG:HB2	1:A:107:ASP:HB3	1.92	0.52
1:B:179:GLU:OE2	1:B:326:LYS:HA	2.09	0.52
1:B:14:LEU:O	1:B:218:SER:OG	2.16	0.52
1:B:153:LEU:C	1:B:153:LEU:HD12	2.30	0.52
1:A:268:LEU:HA	1:A:308:LYS:CE	2.40	0.52
1:B:193:TRP:O	1:B:213:VAL:HG23	2.09	0.52
1:B:199:ILE:CD1	1:B:209:ALA:HB3	2.40	0.52
1:A:162:ASP:CG	1:A:163:LYS:N	2.63	0.52
1:A:91:ILE:N	1:A:91:ILE:HD12	2.25	0.52
1:A:277:LEU:CD1	1:A:286:MET:H	2.23	0.52
1:A:49:SER:O	1:A:52:CYS:HB2	2.10	0.52
1:B:219:THR:CG2	1:B:288:TYR:CD2	2.93	0.52
1:B:210:ASN:N	1:B:297:ASN:O	2.41	0.52
1:A:257:LEU:HB3	1:A:259:PHE:CZ	2.45	0.51
1:B:206:MET:SD	1:B:297:ASN:OD1	2.68	0.51
1:B:201:PHE:HA	1:B:257:LEU:HD22	1.92	0.51
1:A:174:GLU:HB3	1:A:177:PHE:CD2	2.45	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:178:TYR:OH	1:A:182:LEU:HD22	2.10	0.51
1:A:258:GLU:HB3	1:A:265:LYS:HZ3	1.76	0.51
1:A:260:HIS:HB3	1:A:265:LYS:HB2	1.91	0.51
1:A:155:THR:HG23	1:A:310:PHE:CE1	2.45	0.51
1:A:310:PHE:HB2	1:A:325:ALA:HA	1.91	0.51
1:B:158:LEU:HB2	1:B:307:ARG:HA	1.92	0.51
1:B:251:ASN:CB	1:B:254:LEU:HD11	2.38	0.51
1:A:185:GLU:O	1:A:319:SER:CB	2.56	0.51
1:A:8:LEU:HD11	1:A:156:PHE:HE1	1.75	0.51
1:B:12:ALA:HA	1:B:161:HIS:CE1	2.45	0.51
1:A:157:TYR:HB2	1:A:310:PHE:CD1	2.45	0.51
1:A:162:ASP:CG	1:A:163:LYS:H	2.12	0.51
1:A:294:ILE:HD12	2:C:6:STA:CD1	2.40	0.51
1:B:209:ALA:HA	1:B:297:ASN:HB3	1.92	0.51
1:B:193:TRP:CZ2	1:B:313:PHE:HB3	2.45	0.51
1:A:55:LYS:HD2	1:A:115:TYR:CZ	2.45	0.51
1:B:66:TYR:CG	1:B:67:GLU:N	2.78	0.51
1:A:10:ASP:OD1	1:A:11:VAL:N	2.44	0.51
1:A:242:LEU:HD12	1:A:243:PRO:HB3	1.93	0.51
1:B:157:TYR:O	1:B:158:LEU:HD23	2.11	0.51
1:A:244:LEU:CD1	1:A:286:MET:HE3	2.40	0.50
1:B:256:THR:HG22	1:B:256:THR:O	2.10	0.50
1:A:84:GLY:HA3	1:A:104:GLU:O	2.11	0.50
1:A:219:THR:CG2	1:A:290:LEU:H	2.24	0.50
1:A:280:ILE:N	1:A:280:ILE:HD12	2.26	0.50
1:B:306:MET:C	1:B:308:LYS:H	2.13	0.50
1:A:275:ASP:H	1:A:285:CYS:CB	2.17	0.50
1:A:201:PHE:CD1	1:A:202:GLY:N	2.78	0.50
1:A:192:TYR:HB2	1:A:212:VAL:HG22	1.92	0.50
1:A:294:ILE:HD12	2:C:6:STA:HD11	1.94	0.50
1:A:114:ILE:N	1:A:114:ILE:HD12	2.18	0.50
1:A:138:PRO:HG2	1:A:141:VAL:CG2	2.42	0.50
1:A:201:PHE:HB3	1:A:257:LEU:HA	1.94	0.50
1:B:183:THR:O	1:B:321:GLY:HA2	2.12	0.50
1:A:163:LYS:HD2	1:A:327:ASN:OD1	2.11	0.50
1:A:312:VAL:HB	1:A:321:GLY:HA3	1.93	0.50
1:B:80:GLY:HA3	1:B:111:LEU:CD1	2.41	0.50
1:A:256:THR:HG23	1:A:268:LEU:C	2.33	0.50
1:A:95:ASP:OD2	1:A:96:LEU:HG	2.12	0.50
1:B:152:ALA:HB3	1:B:316:GLU:HG3	1.93	0.50
1:B:236:VAL:HB	1:B:287:LEU:CD2	2.39	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:230:PHE:CE2	1:A:234:MET:SD	3.05	0.49
1:A:277:LEU:HD12	1:A:277:LEU:N	2.27	0.49
1:B:244:LEU:CG	1:B:286:MET:HE1	2.38	0.49
1:B:219:THR:HA	1:B:304:PRO:CD	2.42	0.49
1:A:47:CYS:SG	1:A:49:SER:HB3	2.52	0.49
1:B:206:MET:CG	1:B:209:ALA:HB2	2.41	0.49
1:A:92:SER:O	1:A:93:LEU:HD13	2.12	0.49
1:A:146:GLN:O	1:A:147:ASN:C	2.51	0.49
1:A:275:ASP:OD2	1:A:285:CYS:HB3	2.13	0.49
1:A:314:ASP:CG	1:A:317:LYS:H	2.15	0.49
1:B:301:LEU:HD13	1:B:305:PHE:CD1	2.48	0.49
1:B:50:ILE:N	1:B:50:ILE:HD12	2.28	0.49
1:A:224:THR:HG22	1:A:228:ASN:ND2	2.28	0.49
1:B:294:ILE:HG12	1:B:298:THR:HB	1.93	0.49
1:A:15:MET:C	1:A:16:PHE:CD1	2.86	0.49
1:A:280:ILE:HG22	1:A:280:ILE:O	2.12	0.49
1:A:42:VAL:CG1	1:A:58:TYR:HB2	2.42	0.49
1:B:165:VAL:O	1:B:166:GLY:O	2.31	0.49
1:A:92:SER:C	1:A:93:LEU:HD13	2.33	0.49
1:A:210:ASN:HD22	1:A:298:THR:CG2	2.26	0.49
1:B:231:PHE:CD1	1:B:231:PHE:O	2.66	0.49
1:B:230:PHE:O	1:B:234:MET:HB2	2.13	0.49
1:B:273:TYR:O	1:B:288:TYR:HB2	2.13	0.49
1:A:221:THR:HB	1:A:300:ILE:CB	2.37	0.49
1:A:276:PRO:C	1:A:277:LEU:HD12	2.33	0.49
1:A:277:LEU:HD22	1:A:285:CYS:C	2.33	0.49
1:A:80:GLY:HA3	1:A:111:LEU:HD12	1.94	0.49
1:A:67:GLU:HB3	1:A:88:LYS:HB3	1.94	0.49
1:B:227:LEU:HD22	1:B:291:PRO:CA	2.43	0.49
1:A:25:ASN:HD21	1:A:27:GLN:HG2	1.78	0.48
1:A:20:GLY:HA3	1:A:31:PHE:HD2	1.78	0.48
1:B:272:PHE:O	1:B:307:ARG:NH1	2.45	0.48
1:B:83:ARG:H	1:B:105:VAL:HG13	1.79	0.48
1:A:278:SER:O	1:A:279:ASP:C	2.52	0.48
1:A:310:PHE:H	1:A:325:ALA:N	2.12	0.48
1:A:152:ALA:O	1:A:314:ASP:OD1	2.32	0.48
1:B:178:TYR:HA	1:B:325:ALA:CA	2.31	0.48
1:B:251:ASN:O	1:B:254:LEU:HD13	2.13	0.48
1:B:286:MET:SD	1:B:288:TYR:HE1	2.36	0.48
1:B:303:ASP:N	1:B:304:PRO:CD	2.76	0.48
1:B:305:PHE:CD2	1:B:305:PHE:O	2.65	0.48



		Interatomic	Clash
Atom-1	com-1 Atom-2		overlap (Å)
1:A:13:ASN:HB3	1:A:161:HIS:CA	2.40	0.48
1:B:55:LYS:HB3	1:B:121:ASP:OD1	2.13	0.48
1:B:67:GLU:HB3	1:B:88:LYS:CB	2.43	0.48
1:A:272:PHE:CE2	1:A:308:LYS:HA	2.48	0.48
1:A:178:TYR:CA	1:A:326:LYS:HD2	2.44	0.48
1:A:260:HIS:HB3	1:A:265:LYS:CA	2.44	0.48
1:B:238:LYS:CD	1:B:242:LEU:H	2.26	0.48
1:A:178:TYR:N	1:A:326:LYS:HD2	2.29	0.48
1:B:247:THR:OG1	1:B:287:LEU:HD22	2.13	0.48
1:B:80:GLY:HA3	1:B:111:LEU:HD13	1.96	0.48
1:A:157:TYR:HB2	1:A:310:PHE:CE1	2.49	0.47
1:A:221:THR:HB	1:A:300:ILE:H	1.79	0.47
1:A:83:ARG:HD2	3:A:358:HOH:O	2.14	0.47
1:B:221:THR:HG23	1:B:292:VAL:HB	1.94	0.47
1:A:138:PRO:HG2	1:A:141:VAL:HB	1.96	0.47
1:A:217:THR:HG22	1:A:219:THR:H	1.77	0.47
1:A:239:VAL:HG12	1:A:240:PRO:HD2	1.97	0.47
1:B:201:PHE:O	1:B:255:PRO:HB2	2.14	0.47
1:B:313:PHE:CD1	1:B:313:PHE:N	2.82	0.47
1:A:24:THR:C	1:A:26:LYS:N	2.65	0.47
1:B:276:PRO:O	1:B:278:SER:N	2.46	0.47
1:A:55:LYS:HD2	1:A:115:TYR:OH	2.15	0.47
1:A:98:LEU:N	1:A:98:LEU:HD23	2.29	0.47
1:B:227:LEU:HD11	1:B:289:ILE:CG2	2.43	0.47
1:A:77:TYR:HA	2:C:5:ALA:HA	1.96	0.47
1:A:176:ASP:C	1:A:326:LYS:HD3	2.35	0.47
1:A:220:ILE:HB	1:A:289:ILE:CD1	2.45	0.47
1:B:212:VAL:HG23	1:B:298:THR:HG23	1.97	0.47
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.96	0.47
1:B:39:ASN:HD21	1:B:133:ILE:H	1.62	0.47
1:B:40:LEU:HG	1:B:102:PHE:HB3	1.96	0.47
1:B:69:ASP:HB3	1:B:86:PHE:O	2.15	0.47
1:A:185:GLU:O	1:A:186:LYS:O	2.32	0.47
1:A:160:VAL:C	1:A:162:ASP:H	2.15	0.47
1:A:199:ILE:N	1:A:199:ILE:HD12	2.30	0.47
1:B:196:ASP:HB3	1:B:208:LYS:HD2	1.97	0.47
1:B:244:LEU:HB2	3:B:355:HOH:O	2.15	0.47
1:A:275:ASP:HB3	1:A:276:PRO:HA	1.97	0.47
1:A:302:GLY:HA3	3:A:366:HOH:O	2.15	0.47
1:B:219:THR:O	1:B:302:GLY:HA3	2.15	0.47
1:A:257:LEU:N	1:A:268:LEU:O	2.48	0.46



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:56:HIS:HD2	1:A:121:ASP:OD2	1.99	0.46	
1:B:103:ILE:N	1:B:103:ILE:CD1	2.78	0.46	
1:B:279:ASP:OD1	1:B:280:ILE:HD12	2.16	0.46	
1:B:317:LYS:O	1:B:318:GLU:C	2.54	0.46	
1:A:10:ASP:OD2	1:A:16:PHE:HE2	1.97	0.46	
1:A:245:TYR:O	1:A:287:LEU:HB3	2.15	0.46	
1:B:246:VAL:HG12	1:B:247:THR:H	1.80	0.46	
1:A:280:ILE:CG2	1:B:280:ILE:HG21	2.46	0.46	
1:A:77:TYR:HB3	2:C:4:STA:HD13	1.97	0.46	
1:A:177:PHE:HB3	1:A:310:PHE:CD1	2.51	0.46	
1:A:216:GLY:HA3	2:C:4:STA:OH	2.15	0.46	
1:A:226:PHE:O	1:A:227:LEU:HD12	2.15	0.46	
1:A:145:LYS:C	1:A:147:ASN:H	2.18	0.46	
1:A:220:ILE:CG2	1:A:221:THR:N	2.78	0.46	
1:A:281:ASP:CG	1:B:281:ASP:HB2	2.35	0.46	
1:B:294:ILE:H	1:B:294:ILE:CD1	2.08	0.46	
1:A:22:ILE:HG12	1:A:91:ILE:HG13	1.97	0.46	
1:A:322:PHE:O	1:A:323:ALA:HB2	2.15	0.46	
1:A:67:GLU:CB	1:A:88:LYS:HE2	2.45	0.46	
1:B:140:VAL:HG21	1:B:154:PHE:CD2	2.51	0.46	
1:A:241:PHE:O	1:A:242:LEU:HB3	2.15	0.46	
1:A:260:HIS:ND1	1:A:265:LYS:HD2	2.31	0.46	
1:A:258:GLU:HB3	1:A:265:LYS:NZ	2.31	0.46	
1:B:305:PHE:C	1:B:305:PHE:CD2	2.89	0.46	
1:A:159:PRO:HD3	1:A:165:VAL:O	2.16	0.45	
1:A:198:ASP:HA	1:A:206:MET:O	2.16	0.45	
1:B:12:ALA:O	1:B:14:LEU:HG	2.16	0.45	
1:A:100:TYR:OH	1:A:138:PRO:HA	2.16	0.45	
1:A:192:TYR:HB3	3:A:351:HOH:O	2.15	0.45	
1:A:244:LEU:HD12	1:A:286:MET:CE	2.40	0.45	
1:A:160:VAL:HG13	1:A:307:ARG:HD3	1.97	0.45	
1:A:200:HIS:HB3	1:A:205:VAL:HA	1.96	0.45	
1:A:239:VAL:HG22	1:A:246:VAL:CG1	2.45	0.45	
1:A:268:LEU:HD12	1:A:308:LYS:CE	2.45	0.45	
1:A:81:THR:O	1:A:110:ASP:HB2	2.16	0.45	
1:B:327:ASN:HB2	1:B:328:LEU:H	1.53	0.45	
1:A:222:ALA:HB3	1:A:227:LEU:HD11	1.97	0.45	
1:A:233:ASP:O	1:A:234:MET:HB2	2.16	0.45	
1:B:278:SER:O	1:B:280:ILE:N	2.41	0.45	
1:A:320:VAL:HG12	1:A:321:GLY:N	2.30	0.45	
1:A:326:LYS:C	1:A:328:LEU:H	2.10	0.45	



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlan (Å)
1:B:159:PRO:HB2	1:B:163:LVS:HB3	1.98	0.45
1:A:154:PHE:N	1:A:154:PHE:CD2	2.85	0.45
$1 \cdot A \cdot 160 \cdot VAL \cdot H$	1·A·163·LVS·CE	2.29	0.45
1.B.246.VAL:CG1	1.R.247.THB.H	2.20	0.15
$1 \cdot B \cdot 91 \cdot ILE \cdot HD12$	$1 \cdot B \cdot 91 \cdot IL E \cdot N$	2.31	0.45
$1 \cdot A \cdot 160 \cdot VAL \cdot HG23$	1·A·163·LVS·NZ	2.32	0.45
$1 \cdot A \cdot 219 \cdot THB \cdot HG22$	$1 \cdot A \cdot 220 \cdot ILE \cdot N$	2.32	0.45
1.A.227.LEU.O	$1 \cdot A \cdot 230 \cdot PHE \cdot HB2$	2.02	0.15
1:A:265:LYS:NZ	1:A:267:THB:HG22	2.31	0.45
$1 \cdot B \cdot 259 \cdot PHE \cdot N$	1.B.266.TVB.O	2.31	0.45
1:A:109:ASP:O	$1 \cdot A \cdot 112 \cdot GLU \cdot HG2$	2.16	0.45
1.A.303.ASP.CB	1.A.307.ABG.HH12	2.10	0.19
$1 \cdot B \cdot 101 \cdot LYS \cdot HE3$	1.B.136.ILE.HD11	1.98	0.45
1.B.140.VAL:HG21	$1 \cdot B \cdot 150 \cdot HD \cdot HD 2$	1.80	0.45
1.B.44.SEB.C	1.B.46.ASN.H	2.21	0.15
1.A.231.PHE.C	$1 \cdot A \cdot 233 \cdot A \text{SP} \cdot N$	2.21	0.19
1.A.201.1 HE.C	$1 \cdot A \cdot 241 \cdot PHE \cdot HD2$	1.62	0.45
$\frac{1 \cdot A \cdot 178 \cdot T Y B \cdot O}{1 \cdot A \cdot 178 \cdot T Y B \cdot O}$	1:A:326:LVS:HD2	2.17	0.19
1.A.187.LEU.C	$\frac{1.4.320.213.0022}{1.4.188.4SN.0D1}$	2.55	0.19
$1 \cdot A \cdot 272 \cdot PHE \cdot CE2$	1:A:308:LVS:HB2	2.50	0.11
1.R.202.PHE:HD2	1.R.305.PHE.C	2.32	0.11
$1 \cdot A \cdot 163 \cdot LYS \cdot HD2$	$1 \cdot A \cdot 164 \cdot HIS \cdot NE2$	2.20	0.44
1:B:51:GLV:HA2	$1 \cdot \text{R} \cdot 116 \cdot \text{SER} \cdot \text{HR3}$	2.01	0.11
1:B:304:PRO:HA	1:B:307:ABG:NH1	2.31	0.44
1.B.74.GLU.C	1·B·75·ILE·HD12	2.37	0.44
1:A:134:GLY:O	1:A:135:SER:HB3	2.01	0.44
1:A:219:THB:CG2	1:A:220:ILE:N	2.10	0.44
1:A:260:HIS:N	1:A:260:HIS:HD2	2.33	0.44
1:A:244:LEU:HD22	1:A:289:ILE:H	1.82	0.44
1:A:20:GLY:HA3	1:A:31:PHE:CE2	2.53	0.44
1:A:75:ILE:HD11	1:A:103:ILE:HD12	1.99	0.44
2:D:350:VAL:CG1	2:D:352:STA:HD23	2.47	0.44
1:A:294:ILE:HG22	1:A:295:ASP:H	1.81	0.44
1:A:284:LEU:CD2	1:B:280:ILE:HG23	2.41	0.44
1:B:155:THR:OG1	1:B:312:VAL:HG22	2.18	0.44
1:A:13:ASN:OD1	1:A:14:LEU:CD1	2.66	0.44
1:A:44:SER:C	1:A:46:ASN:N	2.70	0.44
1:B:124:LEU:HD23	1:B:124:LEU:C	2.38	0.44
1:B:210:ASN:O	1:B:298:THR:HG23	2.17	0.44
1:B:22:ILE:HA	1:B:90:VAL:O	2.17	0.44
1:A:186:LYS:HG3	1:A:187:LEU:H	1.82	0.44



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:40:LEU:HA	1:A:123:ILE:O	2.17	0.44
1:B:239:VAL:HG13	1:B:240:PRO:CD	2.44	0.44
1:B:236:VAL:HB	1:B:247:THR:OG1	2.18	0.44
1:A:125:GLY:O	1:A:126:LEU:HG	2.18	0.43
1:A:186:LYS:HG3	1:A:187:LEU:N	2.32	0.43
1:A:276:PRO:O	1:A:277:LEU:HB2	2.18	0.43
1:A:243:PRO:O	1:A:290:LEU:HD21	2.18	0.43
1:B:276:PRO:C	1:B:278:SER:H	2.20	0.43
1:B:179:GLU:OE2	1:B:326:LYS:HB3	2.17	0.43
1:A:13:ASN:HB2	1:A:307:ARG:NH2	2.18	0.43
1:A:165:VAL:HG21	1:A:167:TYR:OH	2.18	0.43
1:A:192:TYR:O	1:A:194:GLN:N	2.51	0.43
1:A:200:HIS:CE1	1:A:258:GLU:OE2	2.71	0.43
1:A:279:ASP:HB2	1:A:280:ILE:HD12	1.99	0.43
1:A:199:ILE:HG21	1:A:299:PHE:CD2	2.53	0.43
1:A:326:LYS:C	1:A:328:LEU:HD12	2.39	0.43
1:A:50:ILE:O	1:A:52:CYS:N	2.50	0.43
1:A:55:LYS:HE2	1:A:55:LYS:HB3	1.75	0.43
1:B:129:LYS:HD3	1:B:137:ASP:OD1	2.18	0.43
1:B:239:VAL:HB	1:B:243:PRO:HB2	1.99	0.43
1:B:305:PHE:CE2	1:B:309:TYR:CD2	3.06	0.43
1:A:153:LEU:HB3	1:A:314:ASP:CB	2.49	0.43
1:A:257:LEU:HB2	1:A:268:LEU:HB3	2.00	0.43
1:A:259:PHE:O	1:A:266:TYR:N	2.35	0.43
1:A:269:GLU:N	1:A:269:GLU:OE1	2.52	0.43
1:A:5:SER:HB2	1:A:167:TYR:HB3	2.01	0.43
1:A:79:SER:HB3	1:A:114:ILE:CG1	2.41	0.43
1:B:197:LEU:HD13	1:B:259:PHE:HB3	2.00	0.43
1:B:271:GLU:HG3	1:B:272:PHE:N	2.33	0.43
1:B:217:THR:HG22	1:B:219:THR:H	1.83	0.43
1:A:197:LEU:HD13	1:A:259:PHE:HB3	2.00	0.43
1:B:223:PRO:O	1:B:224:THR:C	2.57	0.43
1:B:198:ASP:CB	1:B:260:HIS:HB2	2.35	0.43
1:B:41:TRP:CE3	1:B:105:VAL:HG21	2.54	0.43
1:B:165:VAL:O	1:B:165:VAL:CG1	2.65	0.43
1:A:178:TYR:CZ	1:A:182:LEU:HD22	2.54	0.43
1:B:199:ILE:HG23	1:B:259:PHE:CE1	2.54	0.43
1:B:242:LEU:HD23	1:B:243:PRO:N	2.33	0.43
1:A:128:TRP:CZ2	1:A:315:TYR:HA	2.54	0.43
1:B:149:ILE:HG13	1:B:171:GLY:HA2	2.01	0.43
1:B:286:MET:SD	1:B:288:TYR:CE1	3.12	0.43



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:290:LEU:HD11	2:D:349:IVA:HG22	2.00	0.43	
1:A:3:ASN:ND2	1:A:172:GLY:H	2.17	0.42	
1:A:188:ASN:O	1:A:189:HIS:ND1	2.51	0.42	
1:A:278:SER:O	1:A:281:ASP:N	2.52	0.42	
1:A:309:TYR:HD1	1:A:324:VAL:HA	1.84	0.42	
1:A:178:TYR:CD2	1:A:323:ALA:CB	3.03	0.42	
1:B:184:TYR:HD1	1:B:319:SER:HG	1.67	0.42	
1:B:14:LEU:HD23	1:B:288:TYR:CZ	2.55	0.42	
1:A:73:VAL:CG2	1:A:103:ILE:HD13	2.48	0.42	
1:B:221:THR:CG2	1:B:300:ILE:HG12	2.49	0.42	
1:A:182:LEU:HD12	1:A:323:ALA:CB	2.50	0.42	
1:A:201:PHE:HB3	1:A:257:LEU:HD23	2.02	0.42	
1:B:14:LEU:HB3	1:B:288:TYR:HE2	1.84	0.42	
1:B:241:PHE:C	1:B:243:PRO:CD	2.88	0.42	
1:B:209:ALA:HB1	1:B:297:ASN:O	2.19	0.42	
1:B:15:MET:CE	2:D:350:VAL:HG21	2.48	0.42	
1:A:200:HIS:CE1	1:A:260:HIS:NE2	2.88	0.42	
1:B:191:LEU:HB3	1:B:192:TYR:HD1	1.83	0.42	
1:A:320:VAL:HG11	1:A:322:PHE:CE2	2.54	0.42	
1:B:221:THR:HG21	1:B:300:ILE:HG12	2.02	0.42	
1:A:190:ASP:O	1:A:191:LEU:HD22	2.19	0.42	
1:A:221:THR:HG23	1:A:292:VAL:HB	1.99	0.42	
1:A:303:ASP:O	1:A:306:MET:N	2.53	0.42	
1:B:69:ASP:HB2	1:B:88:LYS:NZ	2.34	0.42	
1:B:19:GLU:CD	1:B:19:GLU:N	2.60	0.42	
1:B:220:ILE:HA	1:B:300:ILE:O	2.20	0.42	
1:B:306:MET:C	1:B:308:LYS:N	2.73	0.42	
1:A:278:SER:C	1:A:280:ILE:N	2.70	0.42	
1:A:277:LEU:HD22	1:A:285:CYS:CA	2.49	0.42	
1:A:80:GLY:CA	1:A:111:LEU:HD12	2.50	0.42	
1:B:254:LEU:N	1:B:254:LEU:CD1	2.81	0.42	
1:B:256:THR:CG2	1:B:269:GLU:HG3	2.50	0.42	
1:B:49:SER:O	1:B:52:CYS:HB2	2.20	0.42	
1:A:12:ALA:O	1:A:14:LEU:CD1	2.60	0.41	
1:A:199:ILE:HG21	1:A:299:PHE:CE2	2.55	0.41	
1:A:262:ARG:HA	3:A:362:HOH:O	2.19	0.41	
1:A:277:LEU:HD13	1:A:286:MET:N	2.35	0.41	
1:A:295:ASP:O	1:A:296:ASP:CB	2.67	0.41	
1:A:67:GLU:HB3	1:A:88:LYS:HE2	2.01	0.41	
1:B:151:ASN:HB2	1:B:171:GLY:O	2.20	0.41	
1:A:14:LEU:HB3	1:A:218:SER:HB2	2.02	0.41	



		Interatomic	Clash overlap (Å)	
Atom-1	Atom-2	distance (Å)		
1:A:278:SER:O	1:A:280:ILE:N	2.52	0.41	
1:A:244:LEU:HD22	1:A:288:TYR:HA	1.98	0.41	
1:B:66:TYR:CD1	1:B:67:GLU:N	2.87	0.41	
1:A:238:LYS:HD2	1:A:239:VAL:O	2.19	0.41	
1:A:236:VAL:HG13	1:A:247:THR:OG1	2.20	0.41	
1:B:144:LYS:CA	1:B:149:ILE:HG22	2.47	0.41	
1:B:162:ASP:O	1:B:164:HIS:N	2.53	0.41	
1:B:196:ASP:O	1:B:197:LEU:HD23	2.20	0.41	
1:B:302:GLY:C	1:B:304:PRO:HD2	2.40	0.41	
1:A:79:SER:CB	1:A:114:ILE:HG12	2.42	0.41	
1:B:187:LEU:HA	1:B:194:GLN:O	2.20	0.41	
1:B:123:ILE:HD11	2:D:352:STA:HD21	2.01	0.41	
1:A:113:PRO:HG3	1:B:79:SER:HA	2.02	0.41	
1:A:314:ASP:OD2	1:A:317:LYS:CD	2.58	0.41	
1:A:187:LEU:O	1:A:194:GLN:O	2.39	0.41	
1:A:24:THR:O	1:A:26:LYS:N	2.54	0.41	
1:A:25:ASN:ND2	1:A:27:GLN:HG2	2.36	0.41	
1:B:230:PHE:C	1:B:232:ARG:H	2.21	0.41	
1:A:200:HIS:CB	1:A:205:VAL:HA	2.51	0.41	
1:A:14:LEU:O	1:A:218:SER:HB3	2.20	0.41	
1:B:144:LYS:HA	1:B:144:LYS:HD2	1.88	0.41	
1:A:326:LYS:C	1:A:328:LEU:N	2.71	0.41	
1:B:109:ASP:O	1:B:111:LEU:N	2.53	0.41	
1:B:162:ASP:O	1:B:163:LYS:C	2.58	0.41	
1:B:278:SER:C	1:B:280:ILE:H	2.23	0.41	
1:A:128:TRP:CE3	1:A:190:ASP:HB3	2.56	0.41	
1:A:1:SER:O	1:A:3:ASN:OD1	2.39	0.41	
1:A:67:GLU:HB2	1:A:88:LYS:CE	2.51	0.41	
1:B:319:SER:OG	1:B:320:VAL:N	2.52	0.41	
1:B:38:ALA:HB3	1:B:132:SER:HB3	2.03	0.41	
1:A:230:PHE:HA	1:A:230:PHE:HD2	1.74	0.41	
1:A:236:VAL:CG1	1:A:245:TYR:CB	2.92	0.41	
1:B:73:VAL:HG11	1:B:86:PHE:CD2	2.56	0.41	
1:B:274:MET:HA	1:B:286:MET:O	2.20	0.40	
1:A:277:LEU:HD13	1:A:285:CYS:CA	2.44	0.40	
1:A:281:ASP:N	1:A:281:ASP:OD1	2.54	0.40	
1:B:140:VAL:HB	1:B:315:TYR:CE2	2.55	0.40	
1:A:174:GLU:OE2	1:A:176:ASP:OD1	2.38	0.40	
1:A:159:PRO:HA	1:A:164:HIS:HE1	1.86	0.40	
1:A:177:PHE:HB3	1:A:310:PHE:CE1	2.57	0.40	
1:A:200:HIS:HB2	1:A:204:TYR:C	2.41	0.40	



Atom-1	Atom-2	${f Interatomic}\ {f distance}\ ({ m \AA})$	Clash overlap (Å)
1:A:50:ILE:C	1:A:52:CYS:N	2.74	0.40
1:B:149:ILE:HD11	1:B:171:GLY:HA3	2.04	0.40
1:B:155:THR:O	1:B:168:LEU:HA	2.21	0.40
1:B:263:ASN:O	1:B:264:ASN:CB	2.61	0.40
1:B:31:PHE:CZ	1:B:40:LEU:HD11	2.56	0.40
1:B:80:GLY:HA3	1:B:111:LEU:HA	2.02	0.40
1:A:290:LEU:CD2	1:A:291:PRO:HD2	2.46	0.40
1:A:295:ASP:OD2	1:A:296:ASP:OD1	2.39	0.40
1:A:41:TRP:HE1	1:A:123:ILE:HD12	1.87	0.40
1:B:227:LEU:HD22	1:B:291:PRO:CB	2.50	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASP:OD2	1:B:232:ARG:NH2[3_454]	1.23	0.97
1:A:207:GLN:NE2	1:B:233:ASP:O[3_454]	1.59	0.61
1:A:198:ASP:CG	1:B:232:ARG:NH2[3_454]	1.64	0.56
1:A:145:LYS:CE	1:B:163:LYS:NZ[5_665]	1.97	0.23
1:A:134:GLY:CA	$1:B:282:PRO:CB[5_665]$	2.01	0.19
1:A:68:LYS:O	1:B:64:LYS:O[2_665]	2.15	0.05
1:A:72:LYS:NZ	1:A:248:THR:OG1[5_665]	2.17	0.03
1:A:198:ASP:OD2	1:B:232:ARG:CZ[3_454]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	326/328~(99%)	251 (77%)	53 (16%)	22~(7%)	1 3
1	В	326/328~(99%)	259~(79%)	43 (13%)	24 (7%)	1 2
2	С	3/6~(50%)	2~(67%)	1 (33%)	0	100 100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percei	ntiles
2	D	3/6~(50%)	3~(100%)	0	0	100	100
All	All	658/668~(98%)	515 (78%)	97~(15%)	46 (7%)	1	3

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	15	MET
1	А	181	PRO
1	А	186	LYS
1	А	276	PRO
1	А	327	ASN
1	В	159	PRO
1	В	161	HIS
1	В	163	LYS
1	В	166	GLY
1	В	242	LEU
1	В	243	PRO
1	В	278	SER
1	В	279	ASP
1	В	296	ASP
1	А	10	ASP
1	А	162	ASP
1	А	241	PHE
1	А	296	ASP
1	В	4	ASP
1	В	110	ASP
1	В	176	ASP
1	В	230	PHE
1	В	264	ASN
1	В	277	LEU
1	А	51	GLY
1	А	61	SER
1	А	275	ASP
1	А	294	ILE
1	В	109	ASP
1	В	208	LYS
1	В	232	ARG
1	В	240	PRO
1	В	280	ILE
1	А	139	VAL
1	А	146	GLN
1	А	234	MET



Mol	Chain	Res	Type
1	А	281	ASP
1	А	324	VAL
1	В	224	THR
1	В	233	ASP
1	А	187	LEU
1	А	242	LEU
1	В	66	TYR
1	А	165	VAL
1	В	202	GLY
1	А	114	ILE

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	293/293~(100%)	261~(89%)	32 (11%)	6 19		
1	В	293/293~(100%)	260~(89%)	33 (11%)	6 18		
2	С	2/2~(100%)	2~(100%)	0	100 100		
2	D	2/2~(100%)	2~(100%)	0	100 100		
All	All	590/590~(100%)	525~(89%)	65~(11%)	6 19		

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	13	ASN
1	А	16	PHE
1	А	40	LEU
1	А	54	THR
1	А	93	LEU
1	А	136	ILE
1	А	155	THR
1	А	164	HIS
1	А	178	TYR
1	А	181	PRO
1	А	183	THR



Mol	Chain	Res	Type
1	А	188	ASN
1	А	195	ILE
1	А	225	SER
1	А	230	PHE
1	А	232	ARG
1	А	235	ASN
1	А	239	VAL
1	А	241	PHE
1	А	243	PRO
1	А	247	THR
1	А	249	CYS
1	А	251	ASN
1	А	260	HIS
1	A	262	ARG
1	A	263	ASN
1	A	269	GLU
1	А	279	ASP
1	А	281	ASP
1	А	304	PRO
1	А	308	LYS
1	А	317	LYS
1	В	3	ASN
1	В	14	LEU
1	В	17	TYR
1	В	19	GLU
1	В	40	LEU
1	В	44	SER
1	В	72	LYS
1	В	88	LYS
1	В	155	THR
1	В	156	PHE
1	В	161	HIS
1	В	162	ASP
1	В	164	HIS
1	В	169	THR
1	В	182	LEU
1	В	187	LEU
1	В	188	ASN
1	В	190	ASP
1	В	213	VAL
1	В	221	THR
1	В	231	PHE



Mol	Chain	Res	Type
1	В	236	VAL
1	В	240	PRO
1	В	243	PRO
1	В	244	LEU
1	В	249	CYS
1	В	258	GLU
1	В	294	ILE
1	В	305	PHE
1	В	307	ARG
1	В	308	LYS
1	В	311	THR
1	В	318	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	3	ASN
1	А	13	ASN
1	А	27	GLN
1	А	56	HIS
1	А	147	ASN
1	А	161	HIS
1	А	200	HIS
1	А	228	ASN
1	А	235	ASN
1	А	251	ASN
1	А	263	ASN
1	В	146	GLN
1	В	161	HIS
1	В	188	ASN
1	В	194	GLN
1	В	228	ASN
1	В	235	ASN
1	В	264	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.



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

4 non-standard protein/DNA/RNA residues 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	True	Chain	Dec	Bog Link Bond lengths			Bond angles			
INIOI	туре	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	STA	D	352	2	10, 10, 11	0.99	1 (10%)	9,12,14	1.30	1 (11%)
2	STA	D	354	2	8,11,11	2.63	2 (25%)	7,14,14	1.53	2 (28%)
2	STA	С	4	2	10, 10, 11	1.05	1 (10%)	9,12,14	1.70	2 (22%)
2	STA	С	6	2	8,11,11	2.59	3 (37%)	7,14,14	1.82	2 (28%)

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	STA	D	352	2	-	2/11/11/12	-
2	STA	D	354	2	-	0/10/12/12	-
2	STA	С	4	2	-	2/11/11/12	-
2	STA	С	6	2	-	0/10/12/12	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
2	D	354	STA	CH-CA	5.51	1.58	1.53
2	С	6	STA	CH-CA	5.50	1.58	1.53
2	D	354	STA	OH-CH	4.55	1.53	1.43
2	С	6	STA	OH-CH	3.78	1.51	1.43
2	С	4	STA	CH-CA	3.19	1.56	1.53
2	D	352	STA	CH-CA	2.74	1.56	1.53
2	С	6	STA	CA-N	2.06	1.54	1.47

All (7) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	С	4	STA	OH-CH-CM	-3.61	101.34	109.08
2	С	6	STA	CM-CH-CA	-3.35	107.67	112.94
2	С	6	STA	OH-CH-CM	2.96	115.08	109.57
2	D	354	STA	OH-CH-CM	2.79	114.77	109.57
2	D	352	STA	OH-CH-CM	-2.78	103.12	109.08
2	С	4	STA	CG-CB-CA	2.20	120.55	115.82
2	D	354	STA	CM-CH-CA	-2.07	109.68	112.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	352	STA	CH-CA-CB-CG
2	С	4	STA	CH-CA-CB-CG
2	D	352	STA	O-C-CM-CH
2	С	4	STA	O-C-CM-CH

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	\mathbf{Res}	Type	Clashes	Symm-Clashes
2	D	352	STA	3	0
2	С	4	STA	5	0
2	С	6	STA	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

