

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1LYW
Title	:	CATHEPSIN D AT PH 7.5
Authors	:	Lee, A.Y.; Gulnik, S.V.; Erickson, J.W
osited on	:	1998-06-30
esolution	:	2.50 Å(reported)
	PDB ID Title Authors osited on esolution	PDB ID : Title : Authors : osited on : esolution :

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 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231(2.50-2.50)
Sidechain outliers	138945	5233(2.50-2.50)

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	97	57%	35%	6% •
1	С	97	45%	51%	••
1	Е	97	57%	37%	• •
1	G	97	49%	39%	9% •
2	В	241	59%	38%	•
2	D	241	56%	38%	5% •
2	F	241	47%	50%	•
2	Н	241	52%	44%	•



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
3	EPE	С	98	-	-	Х	-
3	EPE	G	98	-	-	Х	-



1LYW

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14242 atoms, of which 3296 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			Aton	ıs			ZeroOcc	AltConf	Trace
1	1 A 95	05	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	л	90	890	471	153	117	144	5	0	0	0
1	C	05	Total	С	Η	Ν	0	S	0	0	Ο
1		90	890	471	153	117	144	5	0		U
1	F	05	Total	С	Η	Ν	0	S	0	0	Ο
1		90	890	471	153	117	144	5	0	0	0
1	C	05	Total	С	Η	Ν	Ο	S	0	0	0
	G	30	890	471	153	117	144	5			U

• Molecule 1 is a protein called CATHEPSIN D.

• Molecule 2 is a protein called CATHEPSIN D.

Mol	Chain	Residues			Aton	ıs			ZeroOcc	AltConf	Trace
9	2 B 241	941	Total	С	Η	Ν	Ο	S	0	0	0
	D		2235	1184	390	302	348	11	0	0	U
0	П	941	Total	С	Η	Ν	0	S	0	0	0
		241	2235	1184	390	302	348	11			0
0	Б	941	Total	С	Η	Ν	Ο	S	0	0	0
	Г	241	2235	1184	390	302	348	11	0		0
0	о и	9.41	Total	С	Η	Ν	Ο	S	0	0	0
	11		2235	1184	390	302	348	11			

• Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).





Mol	Chain	Residues		A	ton	ns			ZeroOcc	AltConf
3	2 Λ	1	Total	С	Η	Ν	Ο	S	0	0
	л		17	8	2	2	4	1	0	0
3	C	1	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
່ <u>ບ</u>	U	T	17	8	2	2	4	1		
3	F	1	Total	С	Η	Ν	Ο	\mathbf{S}	0	0
J J		L	17	8	2	2	4	1	0	0
2 C	1	Total	С	Η	Ν	Ο	S	0	0	
0	G		17	8	2	2	4	1		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	55	Total H O 165 110 55	0	0
4	В	110	Total H O 330 220 110	0	0
4	С	55	Total H O 165 110 55	0	0
4	D	78	Total H O 234 156 78	0	0
4	Е	46	Total H O 138 92 46	0	0
4	F	90	Total H O 270 180 90	0	0
4	G	39	Total H O 117 78 39	0	0
4	Н	85	Total H O 255 170 85	0	0



Residue-property plots (i) 3

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: CATHEPSIN D





• Molecule 2: CATHEPSIN D





F115 6116 6116 7119 7119 7120 7121 7126 7124 7126 7126 7126 7128 7128 D132 0132 0133 1134 1135 S143 V144 N145 N145 **N146** V147 F151 D155 D155 D155 D155 D155 Q155 Q155 D161 D161 D161 D161 T164 F165 <mark>G106</mark> G107 V108 K109 V110 E111 R112 R112 G179 E180 L210 D211 0211 0215 1220 L219 L219 L221 C222 C222 C226 E227 A228 1229 V230 V230 D231 T232 r244 E246 E246 L247 Q248 K249 A253 V254 V255 V255 V255 C255 C255 L181 M182 <mark>S 196</mark> <mark>Y 197</mark> L 198 W206 Y261 M262 1237 1238 123 24: R20 7290 (1301) (1301) (1301) (1301) (1311) (1311) (1311) (1311) (1311) (1311) (1311) (1311) (1311) (1311) (1311) (1311) (1312) (131 Y283 K284 L285 R335 <mark>N338</mark> R339 V340 G341 F342 <mark>A343</mark> A346



4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 2	Depositor	
Cell constants	140.26Å 136.80Å 140.42Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	8.00 - 2.50	Depositor	
% Data completeness	73.0 (8.00-2.50)	Depositor	
(in resolution range)	15.0 (0.00 2.00)		
R_{merge}	0.11	Depositor	
R_{sym}	0.11	Depositor	
Refinement program	X-PLOR 3.1	Depositor	
R, R_{free}	0.195 , 0.257	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	14242	wwPDB-VP	
Average B, all atoms $(Å^2)$	16.0	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: EPE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bo	nd lengths	B	ond angles
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.46	0/759	0.78	1/1034~(0.1%)
1	С	0.47	0/759	0.78	0/1034
1	Е	0.51	0/759	0.79	2/1034~(0.2%)
1	G	0.50	0/759	0.84	0/1034
2	В	0.56	0/1884	0.83	4/2551~(0.2%)
2	D	0.58	1/1884~(0.1%)	0.91	10/2551~(0.4%)
2	F	0.58	2/1884~(0.1%)	0.85	6/2551~(0.2%)
2	Н	0.55	0/1884	0.88	9/2551~(0.4%)
All	All	0.55	3/10572~(0.0%)	0.85	32/14340~(0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	Ideal(Å)
2	D	335	ARG	CZ-NH1	6.71	1.41	1.33
2	F	335	ARG	CZ-NH1	5.72	1.40	1.33
2	F	202	ARG	CZ-NH2	5.22	1.39	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
2	D	301	LEU	CB-CG-CD2	-8.75	96.12	111.00
2	F	276	LEU	CB-CG-CD2	-8.02	97.36	111.00
2	D	321	LEU	CB-CG-CD1	7.39	123.56	111.00
2	Н	135	LEU	CB-CG-CD1	-7.14	98.87	111.00
2	D	321	LEU	CB-CG-CD2	-7.04	99.03	111.00
2	D	169	LEU	CB-CG-CD1	-7.01	99.09	111.00
2	Н	127	ILE	CG1-CB-CG2	-6.49	97.12	111.40
1	Ε	51	ILE	CG1-CB-CG2	-6.41	97.29	111.40
2	D	198	LEU	CB-CG-CD2	-6.28	100.33	111.00
2	F	318	LEU	CB-CG-CD1	-6.28	100.32	111.00



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Н	164	ILE	CG1-CB-CG2	-6.24	97.68	111.40
2	D	154	LEU	CB-CG-CD2	-6.14	100.56	111.00
2	D	301	LEU	CB-CG-CD1	6.01	121.22	111.00
2	F	276	LEU	CB-CG-CD1	6.01	121.21	111.00
2	F	321	LEU	CB-CG-CD1	-5.97	100.85	111.00
2	Н	301	LEU	CB-CG-CD1	-5.75	101.22	111.00
1	А	83	LEU	CB-CG-CD2	-5.60	101.47	111.00
2	D	256	LEU	CB-CG-CD1	-5.52	101.62	111.00
2	В	183	LEU	CB-CG-CD1	-5.49	101.68	111.00
2	F	256	LEU	CB-CG-CD1	-5.45	101.74	111.00
2	В	247	LEU	CB-CG-CD1	-5.44	101.75	111.00
2	Н	237	MET	N-CA-C	-5.41	96.40	111.00
2	D	154	LEU	CB-CG-CD1	5.30	120.00	111.00
2	Н	169	LEU	CB-CG-CD1	-5.24	102.08	111.00
2	Н	135	LEU	CB-CG-CD2	5.24	119.91	111.00
2	D	237	MET	N-CA-C	-5.24	96.86	111.00
2	Н	321	LEU	CB-CG-CD1	5.23	119.89	111.00
2	Н	276	LEU	CB-CG-CD2	-5.23	102.12	111.00
2	F	318	LEU	CA-CB-CG	5.18	127.21	115.30
1	Е	83	LEU	CB-CG-CD2	-5.13	102.27	111.00
2	В	259	GLY	N-CA-C	5.11	125.88	113.10
2	В	237	MET	N-CA-C	-5.07	97.32	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	737	153	690	37	0
1	С	737	153	690	56	0
1	Е	737	153	690	40	0
1	G	737	153	690	49	0
2	В	1845	390	1850	88	0
2	D	1845	390	1850	83	0
2	F	1845	390	1850	88	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Н	1845	390	1850	92	0
3	А	15	2	18	4	0
3	С	15	2	18	8	0
3	Е	15	2	18	2	0
3	G	15	2	18	11	0
4	А	55	110	0	0	0
4	В	110	220	0	0	0
4	С	55	110	0	2	0
4	D	78	156	0	0	0
4	Е	46	92	0	0	0
4	F	90	180	0	2	0
4	G	39	78	0	0	0
4	Н	85	170	0	2	0
All	All	10946	3296	10232	451	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 22.

All (451) 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	${ m distance}~({ m \AA})$	overlap (Å)
1:G:7:LEU:HD11	2:H:309:MET:HG2	1.29	1.05
2:H:253:ALA:HB1	2:H:261:TYR:HB3	1.39	1.04
1:E:43:SER:HB2	2:F:117:GLU:HG2	1.39	1.03
1:G:83:LEU:HD23	3:G:98:EPE:H92	1.42	1.02
2:B:172:ASP:HB2	2:B:173:PRO:HD3	1.44	1.00
2:F:293:LYS:HE2	2:F:302:CYS:SG	2.09	0.93
1:E:78:TYR:OH	2:F:122:PRO:HB3	1.77	0.85
1:A:7:LEU:HD22	2:B:307:MET:HG2	1.60	0.84
2:B:230:VAL:HG12	2:B:326:ILE:HD11	1.60	0.84
2:D:264:PRO:HD2	2:D:267:LYS:HD3	1.61	0.83
2:F:264:PRO:HB2	2:F:267:LYS:HG2	1.59	0.81
2:D:200:VAL:HG12	2:D:338:ASN:O	1.80	0.81
1:G:43:SER:HB2	2:H:117:GLU:HB3	1.63	0.81
2:F:263:ILE:HG21	2:F:271:LEU:HD11	1.63	0.80
1:E:68:VAL:HB	1:E:89:GLN:HB3	1.65	0.78
2:B:249:LYS:HA	2:B:249:LYS:HE3	1.66	0.77
2:F:221:LEU:HD11	2:F:247:LEU:HB2	1.67	0.77
2:B:263:ILE:HG21	2:B:271:LEU:HD11	1.66	0.77
1:E:78:TYR:HE1	1:E:80:SER:HB2	1.50	0.76
1:G:7:LEU:HD21	2:H:309:MET:HE2	1.67	0.76



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:B:228:ALA:HB1	2:B:321:LEU:HD13	1.68	0.76
1:E:5:GLU:HG3	1:E:78:TYR:HB2	1.67	0.75
1:A:47:LYS:HD2	2:B:120:LYS:HE2	1.69	0.74
2:F:182:MET:HE3	2:F:190:TYR:HE2	1.51	0.74
2:B:260:GLU:HG3	1:C:51:ILE:HD11	1.68	0.74
2:H:154:LEU:HD21	2:H:160:VAL:HG13	1.69	0.74
2:F:198:LEU:HD21	2:F:278:LEU:HD22	1.70	0.74
1:C:7:LEU:HD21	2:D:307:MET:SD	2.29	0.73
2:F:164:ILE:HG22	2:F:334:ASP:HA	1.70	0.72
1:G:76:ILE:HG13	3:G:98:EPE:H101	1.71	0.72
1:A:53:CYS:SG	1:A:58:LYS:HE3	2.30	0.71
2:H:154:LEU:HD21	2:H:160:VAL:CG1	2.21	0.71
2:B:255:PRO:HB3	2:B:261:TYR:CZ	2.26	0.71
1:G:51:ILE:HG12	1:G:55:ILE:HD11	1.71	0.71
1:E:78:TYR:CE1	1:E:80:SER:HB2	2.26	0.70
1:C:38:ASN:HB2	3:C:98:EPE:H91	1.74	0.70
2:D:139:TYR:CE2	2:D:203:LYS:HG2	2.27	0.70
1:A:19:ILE:HG22	1:A:94:VAL:HG13	1.74	0.69
2:B:271:LEU:HB2	2:B:287:PRO:HB3	1.73	0.69
2:H:277:LYS:NZ	2:H:280:GLY:HA2	2.07	0.69
1:A:62:ASP:HB3	1:E:62:ASP:O	1.91	0.69
2:H:256:LEU:HB2	2:H:260:GLU:HG3	1.74	0.69
2:F:161:ASP:O	2:F:162:GLN:HB2	1.92	0.68
2:H:255:PRO:HB3	2:H:261:TYR:CE2	2.28	0.68
2:D:154:LEU:HD12	2:D:159:LEU:HB2	1.75	0.68
2:D:239:GLY:O	2:D:308:GLY:HA2	1.94	0.68
2:B:169:LEU:HG	2:B:171:ARG:HB2	1.75	0.68
1:G:67:TYR:HE1	1:G:88:SER:HB3	1.58	0.68
3:A:98:EPE:H82	2:B:115:PHE:HA	1.75	0.67
2:B:172:ASP:HB2	2:B:173:PRO:CD	2.24	0.67
2:B:281:LYS:HD3	2:B:282:GLY:N	2.10	0.67
2:H:108:VAL:HB	2:H:159:LEU:HD13	1.77	0.67
2:F:295:SER:HA	2:F:300:THR:HA	1.77	0.66
1:C:72:THR:HB	1:C:87:LEU:HD12	1.76	0.66
1:A:16:TYR:CD2	2:B:131:PHE:HE1	2.14	0.66
2:H:278:LEU:HB2	2:H:283:TYR:CE1	2.30	0.66
1:C:15:TYR:HD1	2:D:179:GLY:HA3	1.62	0.65
1:C:39:LEU:O	3:C:98:EPE:H81	1.96	0.65
1:G:7:LEU:HD22	2:H:238:VAL:HG21	1.78	0.64
2:B:293:LYS:HE2	2:B:302:CYS:SG	2.37	0.64
1:C:7:LEU:HD22	2:D:238:VAL:HG21	1.79	0.64



A 4 1		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:G:83:LEU:HD23	3:G:98:EPE:C9	2.24	0.63
2:D:195:LEU:HD23	2:D:343:ALA:HB2	1.81	0.63
2:F:287:PRO:HA	2:F:290:TYR:CE2	2.34	0.63
2:F:212:GLN:HG2	2:F:223:LYS:HA	1.81	0.62
1:G:87:LEU:CD2	3:G:98:EPE:H71	2.29	0.62
2:H:210:LEU:HD23	2:H:226:CYS:SG	2.39	0.62
2:B:168:TYR:CE2	2:B:170:SER:HA	2.35	0.62
2:H:228:ALA:HB1	2:H:321:LEU:HD13	1.81	0.62
2:B:281:LYS:HD3	2:B:282:GLY:H	1.63	0.62
2:F:199:ASN:O	2:F:208:VAL:HG12	1.99	0.62
2:H:176:GLN:N	2:H:177:PRO:HD2	2.14	0.62
2:B:256:LEU:HD22	1:C:49:LEU:HG	1.82	0.62
2:B:278:LEU:HB2	2:B:283:TYR:CE1	2.35	0.62
1:G:16:TYR:HB2	1:G:30:VAL:O	2.00	0.62
2:H:248:GLN:HB3	2:H:253:ALA:HB3	1.82	0.61
2:F:151:PHE:O	2:F:155:MET:HG3	2.01	0.61
2:B:257:ILE:O	2:B:258:GLN:HB2	2.01	0.60
2:D:176:GLN:HG3	2:D:177:PRO:HD2	1.83	0.60
2:D:199:ASN:HA	2:D:339:ARG:HA	1.84	0.60
1:A:76:ILE:HD13	1:A:76:ILE:H	1.67	0.60
1:A:55:ILE:HD12	2:B:129:ALA:CB	2.32	0.60
2:B:169:LEU:C	2:B:171:ARG:H	2.06	0.59
2:F:162:GLN:O	2:F:184:GLY:HA2	2.01	0.59
1:G:39:LEU:HA	2:H:134:ILE:O	2.01	0.59
1:E:76:ILE:HD12	2:F:144:VAL:HG11	1.85	0.59
2:D:182:MET:HE3	2:D:190:TYR:HE2	1.67	0.59
1:G:21:ILE:HG12	1:G:92:VAL:HG22	1.85	0.59
1:C:15:TYR:CE1	2:D:169:LEU:HB2	2.38	0.59
2:F:248:GLN:HB3	2:F:261:TYR:CD2	2.38	0.59
1:G:42:PRO:HB2	1:G:58:LYS:HG3	1.85	0.59
3:C:98:EPE:H21	2:D:144:VAL:HB	1.85	0.59
1:E:5:GLU:CG	1:E:78:TYR:HB2	2.33	0.59
2:H:323:ASP:HA	2:H:326:ILE:HB	1.84	0.59
1:C:4:PRO:HG3	2:D:309:MET:SD	2.43	0.59
2:F:141:ARG:HD3	2:F:203:LYS:O	2.02	0.59
1:G:4:PRO:HD2	1:G:7:LEU:HD12	1.84	0.59
2:B:328:ARG:HD3	2:B:329:TYR:CE1	2.38	0.58
2:F:285:LEU:HD21	2:F:325:PHE:HD1	1.67	0.58
2:B:210:LEU:HD23	2:B:226:CYS:SG	2.44	0.58
2:B:215:VAL:HG21	2:B:219:LEU:HD23	1.84	0.58
2:D:235:SER:O	2:D:324:VAL:HG23	2.03	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:55:ILE:HD13	1:E:55:ILE:H	1.68	0.58
2:D:264:PRO:HB2	2:D:267:LYS:HB3	1.86	0.58
2:F:182:MET:HE3	2:F:190:TYR:CE2	2.36	0.58
2:D:238:VAL:HA	2:D:307:MET:O	2.04	0.58
1:E:67:TYR:HE1	1:E:88:SER:HB3	1.69	0.57
2:H:176:GLN:HA	2:H:176:GLN:HE21	1.68	0.57
1:G:5:GLU:HG3	2:H:126:PHE:HZ	1.69	0.57
2:B:170:SER:O	2:B:172:ASP:N	2.37	0.57
1:E:42:PRO:HG2	1:E:57:HIS:O	2.04	0.57
2:D:157:GLN:HB2	2:D:159:LEU:HG	1.84	0.57
2:D:265:CYS:O	2:D:268:VAL:HB	2.05	0.57
1:E:84:SER:O	2:F:118:ALA:HA	2.04	0.57
2:F:271:LEU:HB2	2:F:287:PRO:HB3	1.86	0.57
2:B:138:ALA:CB	2:B:142:ILE:HD11	2.35	0.56
2:B:182:MET:HE3	2:B:190:TYR:CE2	2.39	0.56
1:G:7:LEU:O	2:H:234:THR:HG23	2.04	0.56
2:H:238:VAL:HG22	2:H:307:MET:HB3	1.88	0.56
2:B:207:GLN:HB2	2:B:229:ILE:HG22	1.86	0.56
1:A:44:ILE:HA	1:A:58:LYS:HD2	1.87	0.56
2:B:263:ILE:HD12	2:B:291:THR:HG23	1.87	0.56
1:E:40:TRP:HB3	3:E:98:EPE:H52	1.88	0.56
1:A:85:GLY:HA3	2:B:117:GLU:O	2.05	0.56
1:A:16:TYR:CD2	2:B:131:PHE:CE1	2.94	0.56
1:C:37:SER:OG	2:D:138:ALA:HB3	2.06	0.56
1:A:11:MET:HG2	2:B:126:PHE:O	2.06	0.56
2:F:198:LEU:HD23	2:F:208:VAL:HG21	1.87	0.56
2:F:258:GLN:HE21	2:F:258:GLN:HA	1.71	0.56
1:G:51:ILE:HG23	1:G:52:ALA:N	2.21	0.56
2:H:211:ASP:HB2	2:H:277:LYS:HB3	1.88	0.56
1:E:42:PRO:HD3	2:F:132:ASP:O	2.05	0.55
1:G:94:VAL:O	2:H:107:GLY:HA3	2.07	0.55
1:C:38:ASN:CG	3:C:98:EPE:H22	2.26	0.55
2:F:258:GLN:NE2	2:F:258:GLN:HA	2.20	0.55
2:D:256:LEU:HB2	2:D:260:GLU:HB2	1.87	0.55
2:D:220:THR:HG22	2:D:223:LYS:HG2	1.88	0.55
1:G:83:LEU:CD2	3:G:98:EPE:H92	2.27	0.55
2:F:144:VAL:HG12	2:F:145:ASN:ND2	2.22	0.55
2:F:241:VAL:HG11	1:G:75:ASP:N	2.21	0.55
2:H:277:LYS:HZ3	2:H:280:GLY:HA2	1.72	0.55
2:B:263:ILE:CG2	2:B:271:LEU:HD11	2.36	$0.\overline{55}$
2:B:164:ILE:HD11	2:B:185:GLY:HA2	1.88	0.54



	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:211:ASP:HB2	2:D:277:LYS:O	2.08	0.54
1:C:77:HIS:HD2	1:C:79:GLY:H	1.55	0.54
2:H:278:LEU:HB2	2:H:283:TYR:HE1	1.71	0.54
2:B:238:VAL:HG22	2:B:307:MET:HB3	1.90	0.54
1:C:7:LEU:HD22	2:D:238:VAL:CG2	2.38	0.54
2:D:228:ALA:HB1	2:D:321:LEU:HD13	1.89	0.54
2:H:110:VAL:CG1	2:H:153:ASN:HB3	2.38	0.54
2:H:229:ILE:CG2	2:H:318:LEU:HD13	2.36	0.54
1:A:7:LEU:HD13	2:B:238:VAL:HG21	1.90	0.53
2:H:285:LEU:HD21	2:H:325:PHE:HA	1.90	0.53
2:F:200:VAL:HA	2:F:207:GLN:O	2.08	0.53
2:F:242:ASP:HA	2:F:245:ARG:NH1	2.24	0.53
1:G:5:GLU:HB3	2:H:126:PHE:CE2	2.43	0.53
2:H:151:PHE:O	2:H:155:MET:HG3	2.09	0.53
2:F:121:GLN:HB2	2:F:122:PRO:HD2	1.90	0.53
1:A:53:CYS:O	1:A:58:LYS:NZ	2.38	0.53
1:C:77:HIS:CD2	1:C:79:GLY:H	2.26	0.53
2:D:213:VAL:HB	2:D:221:LEU:HB2	1.90	0.53
1:E:84:SER:HB2	2:F:120:LYS:HB3	1.91	0.53
1:A:95:PRO:HD2	2:B:107:GLY:HA3	1.90	0.53
2:D:229:ILE:HG23	2:D:318:LEU:HD13	1.90	0.53
2:F:212:GLN:HA	2:F:222:CYS:O	2.09	0.53
1:C:95:PRO:HG2	1:C:97:GLN:OXT	2.10	0.52
1:C:15:TYR:CD1	2:D:179:GLY:HA3	2.43	0.52
1:C:18:GLU:HG3	1:C:28:PHE:O	2.09	0.52
1:C:38:ASN:CB	3:C:98:EPE:H22	2.38	0.52
2:H:256:LEU:HB2	2:H:260:GLU:CG	2.38	0.52
2:F:244:VAL:O	2:F:248:GLN:HG2	2.10	0.52
2:F:251:ILE:O	2:F:271:LEU:HD22	2.09	0.52
2:B:165:PHE:HA	2:B:182:MET:O	2.10	0.52
1:C:22:GLY:HA2	1:C:90:ASP:OD1	2.09	0.52
2:H:124:ILE:HA	2:H:127:ILE:O	2.10	0.52
2:D:266:GLU:CD	2:D:266:GLU:H	2.13	0.52
2:H:144:VAL:O	2:H:147:VAL:HG23	2.09	0.52
1:C:4:PRO:HG2	1:C:7:LEU:HD12	1.92	0.52
2:H:268:VAL:HA	2:H:271:LEU:HD13	1.91	0.52
1:C:75:ASP:O	1:C:76:ILE:HD13	2.10	0.51
2:F:241:VAL:HG21	1:G:75:ASP:HB2	1.92	0.51
1:G:47:LYS:O	1:G:48:LEU:HD23	2.10	0.51
2:B:166:SER:O	2:B:181:LEU:HA	2.09	0.51
2:B:221:LEU:HD11	2:B:247:LEU:HB2	1.93	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:51:ILE:O	1:A:55:ILE:HG12	2.10	0.51
1:A:16:TYR:OH	2:B:177:PRO:HB2	2.11	0.51
1:A:55:ILE:HD12	2:B:129:ALA:HB1	1.92	0.51
2:B:297:ALA:HB3	2:D:128:ALA:HB1	1.92	0.51
2:D:262:MET:HE3	2:D:302:CYS:O	2.10	0.51
2:F:148:LEU:HD23	2:F:153:ASN:OD1	2.11	0.51
2:F:293:LYS:CE	2:F:302:CYS:SG	2.93	0.51
2:F:328:ARG:HG3	2:F:329:TYR:CD2	2.46	0.51
3:C:98:EPE:C2	2:D:144:VAL:HB	2.40	0.51
2:B:148:LEU:HD12	2:B:149:PRO:HD2	1.92	0.51
1:E:52:ALA:O	1:E:56:HIS:HB2	2.10	0.51
3:A:98:EPE:H72	2:B:147:VAL:HG11	1.93	0.51
1:C:8:LYS:NZ	1:C:35:GLY:HA3	2.26	0.51
1:G:32:PHE:HB3	2:H:167:PHE:HE2	1.76	0.51
1:C:5:GLU:CD	1:C:5:GLU:H	2.14	0.50
2:H:188:SER:HA	2:H:191:TYR:CE1	2.45	0.50
2:B:248:GLN:HB3	2:B:261:TYR:CD2	2.46	0.50
2:D:315:SER:O	2:D:318:LEU:HD23	2.10	0.50
1:G:82:SER:HB2	2:H:120:LYS:NZ	2.26	0.50
2:H:133:GLY:C	2:H:134:ILE:HD13	2.32	0.50
2:B:182:MET:HE3	2:B:190:TYR:HE2	1.76	0.50
1:C:68:VAL:HB	1:C:89:GLN:HB3	1.94	0.50
1:E:39:LEU:HD12	1:E:40:TRP:H	1.76	0.50
2:D:155:MET:HG2	2:D:163:ASN:CG	2.32	0.50
2:F:278:LEU:HB2	2:F:283:TYR:CE1	2.47	0.50
2:B:166:SER:HB2	2:B:330:TYR:CE1	2.47	0.50
1:A:9:ASN:ND2	2:B:235:SER:HB2	2.27	0.49
2:B:249:LYS:HA	2:B:249:LYS:CE	2.40	0.49
2:B:284:LYS:HG2	2:B:285:LEU:N	2.26	0.49
1:G:38:ASN:OD1	2:H:143:SER:HA	2.12	0.49
2:B:148:LEU:HD11	2:B:152:ASP:HB3	1.93	0.49
2:B:253:ALA:HB1	2:B:261:TYR:HB3	1.94	0.49
2:D:110:VAL:CG1	2:D:153:ASN:HB3	2.42	0.49
2:D:139:TYR:OH	2:D:200:VAL:HG11	2.12	0.49
1:G:77:HIS:O	1:G:79:GLY:N	2.45	0.49
2:H:262:MET:SD	2:H:303:LEU:HB3	2.52	0.49
2:H:264:PRO:HB2	2:H:267:LYS:HB3	1.93	0.49
2:B:240:PRO:O	2:B:244:VAL:HG23	2.12	0.49
2:D:172:ASP:OD1	2:D:173:PRO:HD3	2.12	0.49
2:F:264:PRO:HB2	2:F:267:LYS:CG	2.36	0.49
2:F:234:THR:O	2:F:322:GLY:HA3	2.13	0.49



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:256:LEU:HD12	2:H:260:GLU:HG3	1.95	0.49
1:E:9:ASN:O	1:E:10:TYR:HB2	2.12	0.49
2:F:265:CYS:HA	2:F:268:VAL:HG23	1.94	0.49
1:G:87:LEU:HD21	3:G:98:EPE:H71	1.95	0.49
2:D:163:ASN:O	2:D:335:ARG:HB2	2.11	0.49
1:A:7:LEU:O	2:B:234:THR:HG23	2.13	0.49
2:D:271:LEU:HB3	2:D:272:PRO:HD2	1.95	0.49
2:D:323:ASP:HA	2:D:326:ILE:HB	1.95	0.49
1:E:85:GLY:HA3	2:F:117:GLU:O	2.13	0.49
2:F:164:ILE:HD11	2:F:185:GLY:HA2	1.94	0.49
1:C:5:GLU:HB2	2:D:126:PHE:CZ	2.48	0.48
2:D:173:PRO:C	2:D:175:ALA:H	2.17	0.48
2:D:221:LEU:HD11	2:D:247:LEU:HB2	1.95	0.48
1:G:10:TYR:N	1:G:10:TYR:CD1	2.80	0.48
2:H:157:GLN:O	2:H:159:LEU:N	2.46	0.48
2:D:212:GLN:HA	2:D:222:CYS:O	2.13	0.48
2:F:331:THR:HG23	2:F:342:PHE:CE1	2.48	0.48
2:B:311:ILE:O	2:B:316:GLY:HA3	2.13	0.48
1:C:8:LYS:HZ3	1:C:35:GLY:HA3	1.79	0.48
1:C:9:ASN:O	1:C:10:TYR:HB2	2.13	0.48
2:D:278:LEU:HB2	2:D:283:TYR:CE1	2.47	0.48
2:B:228:ALA:HB1	2:B:321:LEU:CD1	2.43	0.48
1:E:14:GLN:HG2	2:F:323:ASP:OD2	2.13	0.48
3:C:98:EPE:H21	2:D:144:VAL:CB	2.42	0.48
2:D:168:TYR:OH	2:D:170:SER:HB3	2.13	0.48
2:D:264:PRO:O	2:D:267:LYS:HB3	2.14	0.48
2:F:182:MET:CE	2:F:190:TYR:HE2	2.23	0.48
1:G:39:LEU:O	3:G:98:EPE:H52	2.13	0.48
1:A:39:LEU:O	3:A:98:EPE:H81	2.13	0.48
2:D:154:LEU:CD1	2:D:159:LEU:HB2	2.43	0.48
2:D:182:MET:HE3	2:D:190:TYR:CE2	2.48	0.48
1:C:67:TYR:CZ	1:C:69:LYS:HA	2.49	0.48
1:C:40:TRP:HB3	3:C:98:EPE:H52	1.95	0.48
1:E:14:GLN:O	2:F:178:GLY:HA2	2.13	0.48
1:E:6:VAL:HG21	1:G:77:HIS:NE2	2.28	0.48
2:D:211:ASP:O	2:D:225:GLY:HA2	2.13	0.48
2:H:330:TYR:HB3	2:H:343:ALA:HB3	1.95	0.47
1:C:87:LEU:HA	2:D:115:PHE:O	2.13	0.47
1:C:4:PRO:HG3	2:D:309:MET:CE	2.44	0.47
1:G:42:PRO:HD3	2:H:132:ASP:O	2.13	0.47
3:A:98:EPE:C8	2:B:115:PHE:HA	2.41	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
2:B:229:ILE:O	2:B:229:ILE:HG13	2.13	0.47
2:F:253:ALA:HB1	2:F:261:TYR:HB3	1.95	0.47
1:G:5:GLU:HB3	2:H:126:PHE:HE2	1.79	0.47
2:H:196:SER:O	2:H:341:GLY:HA2	2.15	0.47
1:E:54:TRP:HD1	1:E:55:ILE:HG23	1.80	0.47
2:F:196:SER:O	2:F:341:GLY:HA2	2.14	0.47
2:F:278:LEU:HB2	2:F:283:TYR:CD1	2.50	0.47
1:C:10:TYR:CD1	1:C:10:TYR:N	2.83	0.47
2:D:200:VAL:HA	2:D:207:GLN:O	2.14	0.47
1:C:5:GLU:HG3	1:C:78:TYR:O	2.15	0.47
2:H:263:ILE:HD13	2:H:271:LEU:HD21	1.96	0.47
1:C:34:THR:HG23	2:D:232:THR:OG1	2.15	0.47
1:E:40:TRP:HE1	2:F:134:ILE:HD12	1.79	0.47
2:F:211:ASP:HB2	2:F:277:LYS:O	2.15	0.47
2:F:274:ILE:HD12	2:F:306:PHE:CE2	2.50	0.47
1:A:68:VAL:HB	1:A:89:GLN:HB3	1.95	0.46
1:G:7:LEU:HD22	2:H:238:VAL:CG2	2.45	0.46
1:C:31:VAL:HB	2:D:134:ILE:HG13	1.97	0.46
2:D:334:ASP:HB3	2:D:339:ARG:HG2	1.96	0.46
2:H:229:ILE:HG21	2:H:318:LEU:HD13	1.97	0.46
1:A:3:ILE:HD13	2:B:205:TYR:CZ	2.50	0.46
2:F:110:VAL:HG22	2:F:154:LEU:HD12	1.97	0.46
2:B:244:VAL:O	2:B:248:GLN:HG2	2.15	0.46
2:H:230:VAL:HG21	2:H:340:VAL:HG11	1.98	0.46
1:A:61:SER:HB2	1:A:67:TYR:CD2	2.51	0.46
2:B:138:ALA:HB3	2:B:142:ILE:HD11	1.98	0.46
2:H:155:MET:SD	2:H:163:ASN:HB3	2.56	0.46
2:H:198:LEU:HD21	2:H:278:LEU:HB3	1.98	0.46
2:D:197:TYR:O	2:D:198:LEU:HD12	2.16	0.46
1:G:93:SER:HA	2:H:108:VAL:O	2.15	0.46
2:H:162:GLN:O	2:H:184:GLY:HA2	2.15	0.46
2:F:256:LEU:HG	2:F:262:MET:HG2	1.98	0.46
1:C:67:TYR:HE1	1:C:88:SER:HB3	1.81	0.45
2:F:247:LEU:HD11	2:F:274:ILE:HD13	1.97	0.45
1:G:85:GLY:HA2	2:H:119:THR:HG23	1.99	0.45
2:H:144:VAL:HG12	2:H:145:ASN:HD22	1.81	0.45
2:H:221:LEU:HD13	2:H:247:LEU:HD12	1.99	0.45
2:B:152:ASP:O	2:B:155:MET:HB2	2.16	0.45
1:G:15:TYR:OH	2:H:169:LEU:HB2	2.17	0.45
2:H:212:GLN:HA	2:H:222:CYS:HB3	1.98	0.45
2:H:265:CYS:HA	2:H:268:VAL:HG23	1.99	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:264:PRO:HB2	2:D:267:LYS:CB	2.46	0.45
2:F:165:PHE:HA	2:F:182:MET:O	2.17	0.45
1:G:19:ILE:HG22	1:G:94:VAL:HG12	1.97	0.45
1:G:34:THR:HG23	2:H:232:THR:OG1	2.15	0.45
1:A:69:LYS:HG3	1:A:70:ASN:N	2.32	0.45
2:B:169:LEU:O	2:B:171:ARG:N	2.50	0.45
1:C:42:PRO:HB2	1:C:58:LYS:HG2	1.98	0.45
2:H:216:ALA:HB3	2:H:272:PRO:HB2	1.98	0.45
1:A:43:SER:HB2	2:B:117:GLU:HB3	1.99	0.45
2:B:295:SER:HA	2:B:299:LYS:O	2.16	0.45
1:G:85:GLY:HA3	2:H:117:GLU:O	2.17	0.45
2:B:192:LYS:HD2	2:B:344:GLU:CD	2.37	0.45
2:F:222:CYS:SG	2:F:226:CYS:N	2.90	0.45
2:F:224:GLU:HB2	4:F:371:HOH:O	2.16	0.45
1:A:55:ILE:HD12	2:B:129:ALA:HB2	1.99	0.45
1:A:19:ILE:O	1:A:96:CYS:HB2	2.17	0.45
1:C:8:LYS:HE3	4:C:476:HOH:O	2.17	0.45
2:D:196:SER:O	2:D:341:GLY:HA2	2.15	0.45
2:F:244:VAL:HG11	2:F:308:GLY:N	2.32	0.45
1:E:56:HIS:NE2	2:F:131:PHE:O	2.50	0.44
2:F:171:ARG:NH2	2:F:345:ALA:HB3	2.32	0.44
2:H:202:ARG:HH22	2:H:318:LEU:HD21	1.82	0.44
2:H:277:LYS:HZ2	2:H:280:GLY:HA2	1.79	0.44
2:B:207:GLN:CB	2:B:229:ILE:HG22	2.46	0.44
1:A:59:TYR:CE2	2:B:115:PHE:HZ	2.35	0.44
3:G:98:EPE:C8	2:H:115:PHE:HA	2.47	0.44
1:C:11:MET:HB2	4:C:338:HOH:O	2.18	0.44
2:F:110:VAL:CG1	2:F:153:ASN:HB3	2.48	0.44
2:F:187:ASP:OD1	2:F:189:LYS:HG2	2.17	0.44
1:E:37:SER:OG	2:F:138:ALA:HB3	2.17	0.44
1:C:54:TRP:CD1	1:C:55:ILE:HG23	2.53	0.44
2:D:216:ALA:HB3	2:D:272:PRO:HB2	1.99	0.44
1:E:9:ASN:ND2	2:F:235:SER:OG	2.51	0.44
1:E:76:ILE:CD1	2:F:144:VAL:HG11	2.47	0.44
1:C:94:VAL:HG11	2:D:183:LEU:HD11	1.99	0.44
2:H:245:ARG:NH1	2:H:249:LYS:HE3	2.33	0.44
2:B:230:VAL:HG21	2:B:340:VAL:HG11	1.99	0.44
1:C:43:SER:HB2	2:D:117:GLU:HB2	2.00	0.44
2:H:152:ASP:O	2:H:156:GLN:HG3	2.18	0.44
1:G:15:TYR:HD1	2:H:179:GLY:HA3	1.83	0.44
2:H:315:SER:O	2:H:318:LEU:HG	2.18	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:299:LYS:HA	2:D:299:LYS:HD2	1.82	0.43
2:F:216:ALA:HB3	2:F:272:PRO:HB3	2.00	0.43
2:F:312:PRO:HA	2:F:313:PRO:HD3	1.71	0.43
1:G:56:HIS:HE1	4:H:350:HOH:O	2.00	0.43
2:D:223:LYS:NZ	2:D:223:LYS:HB3	2.32	0.43
1:G:51:ILE:CG2	1:G:52:ALA:N	2.81	0.43
2:D:162:GLN:HB2	2:D:184:GLY:O	2.19	0.43
2:D:165:PHE:HA	2:D:182:MET:O	2.18	0.43
2:F:213:VAL:O	2:F:221:LEU:N	2.51	0.43
2:H:176:GLN:N	2:H:177:PRO:CD	2.79	0.43
2:D:210:LEU:HA	2:D:278:LEU:HD23	1.99	0.43
1:E:10:TYR:HB3	2:F:127:ILE:HA	2.00	0.43
1:G:18:GLU:HA	1:G:28:PHE:O	2.18	0.43
3:G:98:EPE:S	3:G:98:EPE:H61	2.58	0.43
2:H:202:ARG:HH22	2:H:318:LEU:HD11	1.82	0.43
1:A:19:ILE:C	1:A:96:CYS:HB2	2.38	0.43
1:G:77:HIS:HE1	1:G:80:SER:O	2.01	0.43
1:G:84:SER:OG	2:H:120:LYS:HB3	2.18	0.43
1:E:18:GLU:HA	1:E:28:PHE:O	2.19	0.43
2:H:202:ARG:NH2	2:H:318:LEU:HD11	2.33	0.43
1:C:94:VAL:O	2:D:107:GLY:HA3	2.18	0.43
3:G:98:EPE:H81	2:H:115:PHE:HA	1.99	0.43
2:H:110:VAL:HG11	2:H:153:ASN:HB3	2.00	0.43
1:A:93:SER:HA	2:B:108:VAL:O	2.19	0.43
1:C:42:PRO:HG2	1:C:56:HIS:HB3	1.99	0.43
1:C:7:LEU:CD2	2:D:307:MET:SD	3.04	0.43
2:F:238:VAL:HA	2:F:307:MET:O	2.18	0.43
1:E:10:TYR:CD1	1:E:10:TYR:N	2.86	0.43
2:H:278:LEU:HD12	2:H:283:TYR:CD1	2.53	0.43
1:A:22:GLY:HA2	1:A:90:ASP:OD1	2.19	0.43
2:B:294:VAL:O	2:B:300:THR:HA	2.18	0.42
2:D:285:LEU:HD23	2:D:328:ARG:HD3	2.01	0.42
2:H:238:VAL:HB	2:H:320:ILE:HB	2.02	0.42
1:C:20:GLY:HA2	1:C:26:GLN:O	2.19	0.42
1:A:9:ASN:C	1:A:11:MET:H	2.23	0.42
2:F:235:SER:HA	2:F:323:ASP:H	1.85	0.42
2:F:256:LEU:HB2	2:F:260:GLU:OE2	2.19	0.42
2:B:283:TYR:CD1	2:B:283:TYR:N	2.87	0.42
2:D:331:THR:HG22	2:D:332:VAL:N	2.35	0.42
1:E:85:GLY:HA2	2:F:119:THR:OG1	2.19	0.42
3:G:98:EPE:H22	3:G:98:EPE:O2S	2.19	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:221:LEU:HD23	2:H:243:GLU:HB3	2.02	0.42
2:B:263:ILE:O	2:B:302:CYS:HB2	2.19	0.42
1:C:85:GLY:HA3	2:D:118:ALA:HA	2.01	0.42
1:C:19:ILE:HG22	1:C:94:VAL:HG22	1.99	0.42
1:G:55:ILE:HG13	2:H:129:ALA:HB1	2.01	0.42
2:B:278:LEU:HD12	2:B:283:TYR:CD1	2.55	0.42
1:C:51:ILE:HA	1:C:51:ILE:HD13	1.92	0.42
1:C:78:TYR:N	1:C:81:GLY:O	2.53	0.42
2:F:111:GLU:N	2:F:157:GLN:HE22	2.18	0.42
2:H:219:LEU:HD12	2:H:220:THR:H	1.85	0.42
1:E:57:HIS:O	1:E:58:LYS:HG3	2.20	0.42
2:H:206:TRP:CH2	2:H:335:ARG:HD2	2.55	0.42
1:A:24:PRO:HA	1:A:25:PRO:HD3	1.92	0.42
2:D:154:LEU:HD11	2:D:160:VAL:HG13	2.02	0.42
2:B:260:GLU:H	2:B:260:GLU:CD	2.24	0.42
1:E:5:GLU:CD	1:E:78:TYR:HB2	2.39	0.42
2:H:312:PRO:HA	2:H:313:PRO:HD3	1.87	0.42
2:B:142:ILE:HG23	2:B:204:ALA:HB1	2.01	0.41
2:D:333:PHE:N	2:D:333:PHE:CD1	2.89	0.41
2:D:181:LEU:HD21	2:D:183:LEU:HD21	2.01	0.41
1:C:52:ALA:O	1:C:56:HIS:HB2	2.20	0.41
2:H:215:VAL:HB	2:H:219:LEU:HB3	2.03	0.41
2:B:169:LEU:C	2:B:171:ARG:N	2.71	0.41
2:D:222:CYS:SG	2:D:226:CYS:N	2.93	0.41
2:F:172:ASP:HA	2:F:173:PRO:HD3	1.91	0.41
1:G:20:GLY:O	1:G:92:VAL:HA	2.21	0.41
2:B:230:VAL:HG12	2:B:326:ILE:CD1	2.39	0.41
2:B:242:ASP:O	2:B:245:ARG:HG2	2.20	0.41
2:B:294:VAL:HG12	2:B:295:SER:N	2.35	0.41
2:B:295:SER:HA	2:B:300:THR:HA	2.03	0.41
2:F:122:PRO:HG2	2:F:127:ILE:HD12	2.02	0.41
2:F:182:MET:CE	2:F:190:TYR:CE2	3.02	0.41
2:F:201:THR:HG22	4:F:435:HOH:O	2.19	0.41
2:F:301:LEU:HD12	2:F:301:LEU:N	2.35	0.41
2:H:169:LEU:HD12	2:H:169:LEU:HA	1.83	0.41
1:C:10:TYR:HD1	1:C:10:TYR:N	2.17	0.41
1:C:19:ILE:O	1:C:27:CYS:HA	2.20	0.41
1:C:67:TYR:OH	1:C:69:LYS:HA	2.20	0.41
1:E:34:THR:HG23	2:F:232:THR:OG1	2.21	0.41
2:H:181:LEU:HD12	2:H:182:MET:H	1.84	0.41
1:E:51:ILE:O	1:E:55:ILE:HD13	$2.\overline{20}$	0.41



Atom 1	A toma D	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:A:55:ILE:HG12	1:A:55:ILE:H	1.69	0.41
2:D:256:LEU:HD11	2:D:262:MET:HG3	2.01	0.41
2:H:112:ARG:HB3	4:H:429:HOH:O	2.20	0.41
2:H:165:PHE:HA	2:H:182:MET:O	2.20	0.41
2:H:254:VAL:O	2:H:261:TYR:HA	2.21	0.41
1:E:17:GLY:N	1:E:32:PHE:CE2	2.89	0.41
2:D:162:GLN:O	2:D:184:GLY:HA2	2.21	0.41
2:D:245:ARG:HB3	2:D:245:ARG:NH1	2.36	0.41
2:F:289:ASP:OD2	2:F:328:ARG:HD2	2.21	0.41
1:A:77:HIS:O	1:A:79:GLY:N	2.54	0.40
2:B:337:ASN:O	2:B:338:ASN:HB2	2.21	0.40
1:C:3:ILE:HD11	2:D:229:ILE:CD1	2.52	0.40
2:B:266:GLU:HG2	2:B:267:LYS:N	2.34	0.40
1:E:94:VAL:HA	1:E:95:PRO:HA	1.77	0.40
1:A:9:ASN:O	1:A:11:MET:N	2.54	0.40
2:B:215:VAL:CG2	2:B:219:LEU:HD23	2.50	0.40
2:D:294:VAL:HG12	2:D:301:LEU:HD13	2.03	0.40
2:H:271:LEU:HB3	2:H:290:TYR:OH	2.21	0.40
1:E:38:ASN:OD1	3:E:98:EPE:H22	2.22	0.40
2:F:140:PRO:HB3	2:F:149:PRO:HD2	2.04	0.40
2:F:142:ILE:HG23	2:F:204:ALA:HB1	2.03	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	Percentiles
1	А	93/97~(96%)	80~(86%)	10 (11%)	3 (3%)	4 5
1	С	93/97~(96%)	83 (89%)	9 (10%)	1 (1%)	14 26
1	Е	93/97~(96%)	83 (89%)	9 (10%)	1 (1%)	14 26
1	G	93/97~(96%)	79 (85%)	12 (13%)	2 (2%)	6 10



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Per	$\operatorname{centiles}$
2	В	239/241~(99%)	209~(87%)	23 (10%)	7(3%)	4	4 6
2	D	239/241~(99%)	215~(90%)	18 (8%)	6 (2%)	, ,	5 8
2	F	239/241~(99%)	218~(91%)	13~(5%)	8 (3%)	4	4 5
2	Н	239/241~(99%)	211 (88%)	24 (10%)	4 (2%)	9	16
All	All	1328/1352~(98%)	1178 (89%)	118 (9%)	32~(2%)	(5 9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	78	TYR
2	В	171	ARG
2	В	173	PRO
1	С	9	ASN
2	D	216	ALA
1	Е	9	ASN
2	F	162	GLN
1	G	78	TYR
2	Н	158	LYS
2	Н	260	GLU
1	А	9	ASN
1	А	79	GLY
2	В	170	SER
2	В	172	ASP
2	D	124	ILE
2	D	268	VAL
2	F	107	GLY
2	F	123	GLY
2	D	172	ASP
2	D	269	SER
2	F	204	ALA
2	Н	338	ASN
2	В	203	LYS
2	D	217	SER
2	F	174	ASP
1	G	10	TYR
2	Н	123	GLY
2	В	107	GLY
2	В	218	GLY
2	F	257	ILE
2	F	218	GLY
2	F	150	VAL



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	84/86~(98%)	76~(90%)	8 (10%)	8 17
1	С	84/86~(98%)	82~(98%)	2(2%)	49 74
1	Ε	84/86~(98%)	78~(93%)	6~(7%)	14 28
1	G	84/86~(98%)	70~(83%)	14 (17%)	2 4
2	В	199/199~(100%)	190~(96%)	9~(4%)	27 51
2	D	199/199~(100%)	189~(95%)	10~(5%)	24 46
2	F	199/199~(100%)	189~(95%)	10~(5%)	24 46
2	Η	199/199~(100%)	$190 \ (96\%)$	9(4%)	27 51
All	All	1132/1140~(99%)	1064 (94%)	68(6%)	19 37

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

Mol	Chain	Res	Type
1	А	29	THR
1	А	41	VAL
1	А	55	ILE
1	А	58	LYS
1	А	72	THR
1	А	76	ILE
1	А	78	TYR
1	А	80	SER
2	В	108	VAL
2	В	130	LYS
2	В	170	SER
2	В	199	ASN
2	В	217	SER
2	В	246	GLU
2	В	249	LYS
2	В	270	THR
2	В	309	MET
1	С	55	ILE
1	С	66	THR



Mol	Chain	Res	Type
2	D	124	ILE
2	D	152	ASP
2	D	160	VAL
2	D	172	ASP
2	D	214	GLU
2	D	258	GLN
2	D	277	LYS
2	D	301	LEU
2	D	303	LEU
2	D	309	MET
1	Е	5	GLU
1	Е	11	MET
1	Е	55	ILE
1	Е	69	LYS
1	Е	93	SER
1	Е	96	CYS
2	F	124	ILE
2	F	135	LEU
2	F	152	ASP
2	F	232	THR
2	F	260	GLU
2	F	266	GLU
2	F	270	THR
2	F	303	LEU
2	F	307	MET
2	F	309	MET
1	G	5	GLU
1	G	23	THR
1	G	29	THR
1	G	44	ILE
1	G	47	LYS
1	G	48	LEU
1	G	55	ILE
1	G	58	LYS
1	G	61	SER
1	G	66	THR
1	G	78	TYR
1	G	93	SER
1	G	94	VAL
1	G	96	CYS
2	Н	112	ARG
2	Н	121	GLN



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Mol	Chain	\mathbf{Res}	Type
2	Н	162	GLN
2	Н	176	GLN
2	Н	241	VAL
2	Н	266	GLU
2	Н	301	LEU
2	Н	303	LEU
2	Н	310	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
2	В	162	GLN
2	В	199	ASN
2	В	337	ASN
2	В	338	ASN
1	С	56	HIS
1	С	77	HIS
2	F	145	ASN
2	F	258	GLN
1	G	56	HIS
1	G	57	HIS
2	Н	145	ASN
2	Н	176	GLN
2	Н	199	ASN
2	Н	258	GLN
2	Н	338	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.



5.6 Ligand geometry (i)

4 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	Chain	Dec	Tinle	Bond lengths			Bond angles												
	туре	Chain	nes	nes	nes	nes	nes	nes	nes	nes	Res	res	res Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	Е	98	-	15, 15, 15	1.25	2 (13%)	$18,\!20,\!20$	2.30	7 (38%)									
3	EPE	G	98	-	15,15,15	0.84	1 (6%)	$18,\!20,\!20$	2.11	7 (38%)									
3	EPE	А	98	-	15,15,15	1.18	2 (13%)	$18,\!20,\!20$	2.52	8 (44%)									
3	EPE	С	98	-	15,15,15	1.36	2 (13%)	$18,\!20,\!20$	2.44	6 (33%)									

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	Е	98	-	-	4/9/19/19	0/1/1/1
3	EPE	G	98	-	-	1/9/19/19	0/1/1/1
3	EPE	А	98	-	-	2/9/19/19	0/1/1/1
3	EPE	С	98	-	-	6/9/19/19	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
3	С	98	EPE	O3S-S	3.69	1.60	1.47
3	Е	98	EPE	O3S-S	3.47	1.59	1.47
3	С	98	EPE	C10-S	3.45	1.82	1.77
3	Е	98	EPE	C10-S	2.93	1.81	1.77
3	А	98	EPE	O3S-S	2.72	1.57	1.47
3	А	98	EPE	C10-S	2.43	1.81	1.77
3	G	98	EPE	O3S-S	2.17	1.55	1.47

All (28) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	Ε	98	EPE	C5-N4-C3	-5.26	96.99	108.83
3	А	98	EPE	O3S-S-C10	4.97	113.80	105.77
3	С	98	EPE	C5-N4-C3	-4.88	97.84	108.83
3	G	98	EPE	O1S-S-C10	4.58	112.44	106.92
3	С	98	EPE	O3S-S-O2S	-4.57	100.11	111.27
3	С	98	EPE	C3-C2-N1	4.44	119.74	110.64
3	А	98	EPE	O1S-S-C10	4.09	111.84	106.92
3	С	98	EPE	O3S-S-C10	4.07	112.34	105.77
3	Е	98	EPE	C9-N1-C2	-4.06	100.86	111.23
3	G	98	EPE	C7-N4-C3	-4.03	100.92	111.23
3	А	98	EPE	C9-N1-C2	4.01	121.50	111.23
3	Е	98	EPE	O3S-S-C10	3.61	111.61	105.77
3	А	98	EPE	O3S-S-O1S	-3.54	102.63	111.27
3	Е	98	EPE	C3-C2-N1	3.23	117.28	110.64
3	А	98	EPE	O3S-S-O2S	-3.13	103.62	111.27
3	С	98	EPE	C5-C6-N1	3.09	116.99	110.64
3	А	98	EPE	C7-N4-C5	-2.93	103.74	111.23
3	Ε	98	EPE	O3S-S-O1S	-2.89	104.21	111.27
3	А	98	EPE	C5-N4-C3	2.85	115.24	108.83
3	G	98	EPE	C6-N1-C2	2.56	114.59	108.83
3	А	98	EPE	C6-N1-C2	2.54	114.55	108.83
3	С	98	EPE	C9-N1-C2	-2.54	104.73	111.23
3	G	98	EPE	O2S-S-C10	-2.50	103.91	106.92
3	Е	98	EPE	O1S-S-C10	2.49	109.91	106.92
3	G	98	EPE	O3S-S-C10	2.48	109.77	105.77
3	Е	98	EPE	C5-C6-N1	2.31	115.38	110.64
3	G	98	EPE	C6-C5-N4	-2.28	105.97	110.64
3	G	98	EPE	O3S-S-O2S	-2.21	105.87	111.27

There are no chirality outliers.

All	(13)	torsion	outliers	are	listed	below:	

Mol	Chain	\mathbf{Res}	Type	Atoms
3	А	98	EPE	C10-C9-N1-C6
3	С	98	EPE	S-C10-C9-N1
3	С	98	EPE	C9-C10-S-O2S
3	С	98	EPE	C9-C10-S-O3S
3	С	98	EPE	C8-C7-N4-C3
3	Е	98	EPE	C9-C10-S-O3S
3	Е	98	EPE	C9-C10-S-O1S
3	Е	98	EPE	C9-C10-S-O2S
3	С	98	EPE	C9-C10-S-O1S
3	С	98	EPE	C8-C7-N4-C5



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Mol	Chain	Res	Type	Atoms
3	Е	98	EPE	C10-C9-N1-C6
3	G	98	EPE	C10-C9-N1-C2
3	А	98	EPE	S-C10-C9-N1

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Ε	98	EPE	2	0
3	G	98	EPE	11	0
3	А	98	EPE	4	0
3	С	98	EPE	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (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.

