

Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2024 – 12:12 PM EST

PDB ID	:	1B6C
Title	:	CRYSTAL STRUCTURE OF THE CYTOPLASMIC DOMAIN OF THE
		TYPE I TGF-BETA RECEPTOR IN COMPLEX WITH FKBP12
Authors	:	Huse, M.; Chen, YG.; Massague, J.; Kuriyan, J.
Deposited on	:	1999-01-13
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The 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
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: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive $(\#Entries)$	Similar resolution $(\#$ Entries, resolution range $(\text{\AA}))$		
Rfree	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	3455 (2.60-2.60)		
Sidechain outliers	138945	3455 (2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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

Mol	Chain	Length	Quality of chain					
1	А	107	74%	26%				
1	С	107	73%	27%				
1	Е	107	^{2%} 74%	26%				
1	G	107	% 7 4%	26%				
2	В	342	3%	31% 6% 5%				



Mol	Chain	Length	Quality of chain					
0	Л	240	5%					
2	D	342	57%	33%	5% 5%			
			9%					
2	F	342	59%	31%	5% 5%			
			4%					
2	Н	342	58%	32%	5% 5%			

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	SO4	F	504	-	-	-	Х



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13840 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Λ	107	Total	С	Ν	Ο	\mathbf{S}	6	0	0
	A	107	831	527	146	154	4	0		
1	С	107	Total	С	Ν	Ο	S	6	0	0
	U	107	831	527	146	154	4	0	0	0
1	F	107	Total	С	Ν	0	S	6	0	0
		107	831	527	146	154	4		0	0
1	1 C	107	Total	С	Ν	0	S	G	0	0
I G	107	831	527	146	154	4	U	0	0	

• Molecule 1 is a protein called FK506-BINDING PROTEIN.

• Molecule 2 is a protein called TGF-B SUPERFAMILY RECEPTOR TYPE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	396	Total	С	Ν	Ο	\mathbf{S}	17	0	0
	D	520	2602	1642	467	477	16	11	0	0
0	Л	206	Total	С	Ν	0	S	17	0	0
	D	320	2602	1642	467	477	16	17		0
0	Б	F 326	Total	С	Ν	0	S	17	0	0
	2 F		2602	1642	467	477	16	17	0	0
0	9 II	200	Total	С	Ν	0	S	17	0	0
	320	2602	1642	467	477	16	11	0	U	

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	D	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	F	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} & \text{O} & \text{S} \\ 5 & 4 & 1 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	2	Total O 2 2	0	0
4	В	20	TotalO2020	0	0
4	С	2	Total O 2 2	0	0
4	D	20	TotalO2020	0	0
4	Е	2	Total O 2 2	0	0
4	F	20	TotalO2020	0	0
4	G	2	Total O 2 2	0	0
4	Н	20	TotalO2020	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: FK506-BINDING PROTEIN







1244 P327 P327 1329 A330 A330 H331 R332 D333 1253 1256 1256 1258 259 260 /321 1322 1323 1324 1326 1326 300 301 1252 310 310 L334 K335 N344 G345 T346 C347 C348 I349 W409 E410 I411 A355 7356 7356 7357 7359 7359 7359 7361 7362 7363 (337 1338 1339 1339 E499 G500 ILE LYS MET E422 D423 Y424 P427



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	75.58Å 81.06 Å 90.53 Å	Deperitor
a, b, c, α , β , γ	86.23° 81.86° 63.92°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	30.00 - 2.60	Depositor
Resolution (A)	19.79 - 2.60	EDS
% Data completeness	98.4 (30.00-2.60)	Depositor
(in resolution range)	90.2 (19.79-2.60)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	$5.60 (at 2.59 \text{\AA})$	Xtriage
Refinement program	CNS 0.3C	Depositor
D D.	0.249 , 0.269	Depositor
Π, Π_{free}	0.248 , 0.266	DCC
R_{free} test set	5883 reflections (10.19%)	wwPDB-VP
Wilson B-factor $(Å^2)$	34.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 12.1	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.230 for -h,-h+k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13840	wwPDB-VP
Average B, all atoms $(Å^2)$	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.26% 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: SO4

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

Mal	Chain	Bo	nd lengths	Bond angles		
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.49	0/850	0.78	0/1146	
1	С	0.48	0/850	0.78	0/1146	
1	Е	0.48	0/850	0.78	0/1146	
1	G	0.48	0/850	0.77	0/1146	
2	В	0.61	1/2655~(0.0%)	0.77	1/3586~(0.0%)	
2	D	0.61	1/2655~(0.0%)	0.77	1/3586~(0.0%)	
2	F	0.62	2/2655~(0.1%)	0.77	2/3586~(0.1%)	
2	H	0.62	1/2655~(0.0%)	0.78	2/3586~(0.1%)	
All	All	0.59	5/14020~(0.0%)	0.77	6/18928~(0.0%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	1
2	D	0	1
2	F	0	1
2	Н	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Н	391	LYS	CG-CD	12.69	1.95	1.52
2	D	391	LYS	CG-CD	12.68	1.95	1.52
2	В	391	LYS	CG-CD	12.68	1.95	1.52
2	F	391	LYS	CG-CD	12.65	1.95	1.52
2	F	283	HIS	C-N	-6.20	1.19	1.34



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Η	391	LYS	CB-CG-CD	-7.56	91.94	111.60
2	D	391	LYS	CB-CG-CD	-7.55	91.96	111.60
2	В	391	LYS	CB-CG-CD	-7.55	91.97	111.60
2	F	391	LYS	CB-CG-CD	-7.53	92.01	111.60
2	Н	283	HIS	O-C-N	6.61	133.27	122.70
2	F	283	HIS	O-C-N	-5.03	114.65	122.70

All (6) bond angle outliers are listed below:

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	424	TYR	Sidechain
2	D	424	TYR	Sidechain
2	F	424	TYR	Sidechain
2	Н	424	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	831	0	831	17	0
1	С	831	0	831	18	0
1	Е	831	0	831	24	0
1	G	831	0	831	17	0
2	В	2602	0	2606	125	0
2	D	2602	0	2606	123	0
2	F	2602	0	2605	127	0
2	Н	2602	0	2606	120	0
3	В	5	0	0	1	0
3	D	5	0	0	1	0
3	F	5	0	0	1	0
3	Н	5	0	0	1	0
4	А	2	0	0	0	0
4	В	20	0	0	0	0
4	C	2	0	0	0	0
4	D	20	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Е	2	0	0	0	0
4	F	20	0	0	0	0
4	G	2	0	0	0	0
4	Н	20	0	0	0	0
All	All	13840	0	13747	545	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 20.

All (545) 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)
2:H:484:THR:HG22	2:H:487:ARG:H	1.28	0.97
2:B:484:THR:HG22	2:B:487:ARG:H	1.28	0.97
2:D:484:THR:HG22	2:D:487:ARG:H	1.28	0.94
2:F:484:THR:HG22	2:F:487:ARG:H	1.28	0.94
2:H:216:PHE:CE2	2:H:372:ARG:HD2	2.04	0.92
2:D:216:PHE:CE2	2:D:372:ARG:HD2	2.07	0.89
2:F:443:LYS:HG2	2:F:448:GLN:HE21	1.39	0.87
2:H:443:LYS:HG2	2:H:448:GLN:HE21	1.39	0.87
2:B:443:LYS:HG2	2:B:448:GLN:HE21	1.39	0.86
2:D:443:LYS:HG2	2:D:448:GLN:HE21	1.39	0.85
1:A:66:MET:HA	1:A:70:GLN:OE1	1.78	0.83
2:B:248:ILE:CD1	2:B:355:ALA:HB3	2.11	0.81
2:B:469:LYS:O	2:B:473:GLU:HG2	1.82	0.80
2:B:193:LEU:CD1	2:B:201:ILE:HD12	2.12	0.80
1:E:66:MET:HA	1:E:70:GLN:OE1	1.82	0.80
2:D:209:GLU:OE2	2:D:221:ARG:NH1	2.16	0.79
2:D:469:LYS:O	2:D:473:GLU:HG2	1.82	0.79
2:F:469:LYS:O	2:F:473:GLU:HG2	1.82	0.79
1:A:88:PRO:HG3	2:B:243:PHE:CD1	2.18	0.79
2:F:193:LEU:CD1	2:F:201:ILE:HD12	2.12	0.79
2:B:209:GLU:OE2	2:B:221:ARG:NH1	2.16	0.79
1:C:66:MET:HA	1:C:70:GLN:OE1	1.82	0.79
2:F:209:GLU:OE2	2:F:221:ARG:NH1	2.16	0.79
2:H:209:GLU:OE2	2:H:221:ARG:NH1	2.16	0.79
2:D:193:LEU:CD1	2:D:201:ILE:HD12	2.12	0.79
2:F:252:VAL:HG11	2:F:329:ILE:HD11	1.65	0.79
1:G:66:MET:HA	1:G:70:GLN:OE1	1.82	0.79
2:H:193:LEU:CD1	2:H:201:ILE:HD12	2.12	0.79
2:H:469:LYS:O	2:H:473:GLU:HG2	1.82	0.79



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:H:409:TRP:HD1	2:H:471:MET:HE1	1.48	0.78
2:D:409:TRP:HD1	2:D:471:MET:HE1	1.49	0.77
2:F:409:TRP:HD1	2:F:471:MET:HE1	1.51	0.76
2:B:409:TRP:HD1	2:B:471:MET:HE1	1.51	0.75
2:F:256:HIS:HD2	2:F:258:ASN:H	1.34	0.75
2:H:256:HIS:HD2	2:H:258:ASN:H	1.35	0.74
2:D:310:ALA:HA	2:D:404:MET:HE1	1.69	0.74
2:H:193:LEU:HD13	2:H:201:ILE:HD12	1.69	0.74
2:B:413:ARG:NH1	2:B:423:ASP:O	2.21	0.74
2:F:413:ARG:NH1	2:F:423:ASP:O	2.21	0.73
2:D:409:TRP:CD1	2:D:471:MET:HE1	2.23	0.73
2:B:256:HIS:HD2	2:B:258:ASN:H	1.35	0.73
2:H:413:ARG:NH1	2:H:423:ASP:O	2.21	0.73
2:D:256:HIS:HD2	2:D:258:ASN:H	1.35	0.73
2:D:413:ARG:NH1	2:D:423:ASP:O	2.21	0.73
2:F:310:ALA:HA	2:F:404:MET:HE1	1.71	0.73
2:D:193:LEU:HD13	2:D:201:ILE:HD12	1.69	0.73
2:B:193:LEU:HD13	2:B:201:ILE:HD12	1.69	0.72
2:F:193:LEU:HD13	2:F:201:ILE:HD12	1.69	0.72
2:B:409:TRP:CD1	2:B:471:MET:HE1	2.24	0.72
2:F:409:TRP:CD1	2:F:471:MET:HE1	2.23	0.72
2:H:331:HIS:HD2	2:H:333:ASP:H	1.37	0.72
2:B:252:VAL:HG11	2:B:329:ILE:HD11	1.72	0.72
2:B:298:THR:HG22	2:B:300:GLU:N	2.05	0.71
2:F:298:THR:HG22	2:F:300:GLU:N	2.05	0.71
2:D:331:HIS:HD2	2:D:333:ASP:H	1.37	0.71
2:F:331:HIS:HD2	2:F:333:ASP:H	1.37	0.71
1:A:88:PRO:HG3	2:B:243:PHE:CE1	2.25	0.71
2:D:298:THR:HG22	2:D:300:GLU:N	2.06	0.71
2:H:409:TRP:CD1	2:H:471:MET:HE1	2.25	0.71
2:H:298:THR:HG22	2:H:300:GLU:N	2.06	0.70
2:F:484:THR:CG2	2:F:487:ARG:H	2.04	0.70
2:B:331:HIS:HD2	2:B:333:ASP:H	1.37	0.70
2:B:216:PHE:HD2	2:B:238:GLU:HG2	1.57	0.69
2:D:216:PHE:HD2	2:D:238:GLU:HG2	1.56	0.69
2:B:484:THR:CG2	2:B:487:ARG:H	2.03	0.69
2:F:216:PHE:HD2	2:F:238:GLU:HG2	1.57	0.69
2:D:484:THR:CG2	2:D:487:ARG:H	2.04	0.69
2:H:216:PHE:HD2	2:H:238:GLU:HG2	1.57	0.69
2:B:248:ILE:HD12	2:B:355:ALA:HB3	1.76	0.68
2:F:283:HIS:CE1	2:F:342:LYS:HG2	2.28	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:88:PRO:HG3	2:H:243:PHE:CE1	2.28	0.68
1:G:88:PRO:HG3	2:H:243:PHE:CD1	2.28	0.68
2:F:184:MET:HE3	2:F:193:LEU:HD22	1.75	0.68
2:B:184:MET:HE3	2:B:193:LEU:HD22	1.76	0.67
2:H:310:ALA:HA	2:H:404:MET:CE	2.25	0.67
2:D:184:MET:HE3	2:D:193:LEU:HD22	1.76	0.67
2:H:484:THR:CG2	2:H:487:ARG:H	2.03	0.67
2:D:310:ALA:HA	2:D:404:MET:CE	2.25	0.67
2:B:310:ALA:HA	2:B:404:MET:CE	2.25	0.67
2:D:309:THR:HG22	2:D:404:MET:HE2	1.76	0.67
2:F:309:THR:HG22	2:F:404:MET:HE2	1.77	0.67
2:H:298:THR:HG22	2:H:301:GLY:H	1.60	0.67
2:F:473:GLU:HB3	2:F:483:LEU:HG	1.77	0.66
1:G:42:ARG:HD2	2:H:184:MET:HG2	1.76	0.66
2:F:298:THR:HG22	2:F:301:GLY:H	1.60	0.66
2:B:298:THR:HG22	2:B:301:GLY:H	1.60	0.66
2:F:269:ASP:HA	2:F:274:THR:HA	1.78	0.66
2:F:310:ALA:HA	2:F:404:MET:CE	2.25	0.66
2:H:473:GLU:HB3	2:H:483:LEU:HG	1.78	0.66
2:D:298:THR:HG22	2:D:301:GLY:H	1.61	0.65
2:H:269:ASP:HA	2:H:274:THR:HA	1.78	0.65
2:B:473:GLU:HB3	2:B:483:LEU:HG	1.77	0.65
2:D:269:ASP:HA	2:D:274:THR:HA	1.78	0.65
2:B:269:ASP:HA	2:B:274:THR:HA	1.78	0.64
2:D:473:GLU:HB3	2:D:483:LEU:HG	1.78	0.64
2:H:184:MET:HE3	2:H:193:LEU:HD22	1.78	0.64
1:E:88:PRO:CB	2:F:246:ALA:HB3	2.28	0.63
1:E:90:ILE:CG1	2:F:250:GLN:HG2	2.28	0.63
2:D:216:PHE:CD2	2:D:238:GLU:HG2	2.34	0.62
1:E:90:ILE:HG13	2:F:250:GLN:HG2	1.79	0.62
2:B:310:ALA:HA	2:B:404:MET:HE1	1.82	0.62
2:H:216:PHE:CD2	2:H:238:GLU:HG2	2.35	0.61
2:B:313:LEU:HB3	2:B:404:MET:HE1	1.82	0.61
2:H:310:ALA:HA	2:H:404:MET:HE1	1.81	0.61
2:H:409:TRP:HB2	2:H:471:MET:HE3	1.82	0.61
2:B:216:PHE:CD2	2:B:238:GLU:HG2	2.35	0.61
2:D:331:HIS:CD2	2:D:333:ASP:H	2.18	0.61
2:F:211:ILE:HD11	2:F:221:ARG:HB2	1.83	0.61
2:H:211:ILE:HD11	2:H:221:ARG:HB2	1.83	0.60
2:B:211:ILE:HD11	2:B:221:ARG:HB2	1.83	0.60
2:D:211:ILE:HD11	2:D:221:ARG:HB2	1.83	0.60



	1.5	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:D:473:GLU:CB	2:D:483:LEU:HG	2.32	0.60
2:F:216:PHE:CD2	2:F:238:GLU:HG2	2.35	0.60
2:H:313:LEU:HB3	2:H:404:MET:HE1	1.82	0.60
2:F:298:THR:HG22	2:F:300:GLU:H	1.67	0.59
2:B:256:HIS:CD2	2:B:258:ASN:H	2.20	0.59
2:B:298:THR:HG22	2:B:300:GLU:H	1.67	0.59
2:H:331:HIS:CD2	2:H:333:ASP:H	2.18	0.59
2:F:331:HIS:CD2	2:F:333:ASP:H	2.18	0.59
2:B:473:GLU:CB	2:B:483:LEU:HG	2.32	0.59
2:F:204:THR:HG22	2:F:204:THR:O	2.02	0.59
2:F:473:GLU:CB	2:F:483:LEU:HG	2.32	0.59
2:H:248:ILE:CD1	2:H:355:ALA:HB3	2.31	0.59
2:H:260:LEU:HD13	2:H:340:LEU:HD12	1.85	0.59
2:H:473:GLU:CB	2:H:483:LEU:HG	2.32	0.59
2:B:204:THR:HG22	2:B:204:THR:O	2.02	0.58
2:D:336:SER:OG	2:D:410:GLU:OE1	2.21	0.58
2:H:377:ARG:HD2	3:H:504:SO4:O2	2.03	0.58
2:D:488:ILE:O	2:D:492:LEU:HB2	2.03	0.58
2:F:256:HIS:CD2	2:F:258:ASN:H	2.19	0.58
2:D:204:THR:O	2:D:204:THR:HG22	2.02	0.58
2:D:377:ARG:HD2	3:D:504:SO4:O2	2.03	0.58
2:F:377:ARG:HD2	3:F:504:SO4:O2	2.03	0.58
2:B:336:SER:OG	2:B:410:GLU:OE1	2.21	0.58
2:H:204:THR:HG22	2:H:204:THR:O	2.02	0.58
2:H:298:THR:HG22	2:H:300:GLU:H	1.68	0.58
2:B:331:HIS:CD2	2:B:333:ASP:H	2.19	0.58
2:H:309:THR:HG22	2:H:404:MET:HE2	1.86	0.58
2:D:232:LYS:HD2	2:D:234:PHE:CZ	2.39	0.57
2:D:298:THR:HG22	2:D:300:GLU:H	1.67	0.57
2:F:488:ILE:O	2:F:492:LEU:HB2	2.04	0.57
1:C:4:VAL:HG22	1:C:74:LEU:HD22	1.87	0.57
2:F:298:THR:CG2	2:F:300:GLU:H	2.18	0.57
2:H:443:LYS:HG2	2:H:448:GLN:NE2	2.17	0.57
2:B:298:THR:CG2	2:B:300:GLU:H	2.17	0.57
2:B:309:THR:HG22	2:B:404:MET:HE2	1.85	0.57
2:B:377:ARG:HD2	3:B:158:SO4:O2	2.03	0.57
2:D:298:THR:CG2	2:D:300:GLU:H	2.18	0.57
2:H:488:ILE:O	2:H:492:LEU:HB2	2.04	0.57
2:B:232:LYS:HD2	2:B:234:PHE:CZ	2.39	0.57
1:E:4:VAL:HG22	1:E:74:LEU:HD22	1.87	0.57
2:F:232:LYS:HD2	2:F:234:PHE:CZ	2.39	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:G:4:VAL:HG22	1:G:74:LEU:HD22	1.87	0.57
2:B:422:GLU:OE1	2:H:434:SER:HB3	2.05	0.57
2:F:336:SER:OG	2:F:410:GLU:OE1	2.21	0.57
2:B:216:PHE:CE2	2:B:372:ARG:HD2	2.40	0.57
2:D:409:TRP:HB2	2:D:471:MET:HE3	1.87	0.57
2:H:336:SER:OG	2:H:410:GLU:OE1	2.21	0.57
2:H:180:LEU:HG	2:H:184:MET:HE2	1.87	0.57
2:H:232:LYS:HD2	2:H:234:PHE:CZ	2.39	0.56
2:B:488:ILE:O	2:B:492:LEU:HB2	2.04	0.56
2:H:256:HIS:CD2	2:H:258:ASN:H	2.20	0.56
2:B:443:LYS:HG2	2:B:448:GLN:NE2	2.17	0.56
1:G:1:GLY:HA2	1:G:80:TYR:CD1	2.41	0.56
2:F:180:LEU:HG	2:F:184:MET:CE	2.36	0.56
2:D:256:HIS:CD2	2:D:258:ASN:H	2.19	0.56
2:B:252:VAL:HG13	2:B:327:PRO:HD2	1.88	0.56
2:H:298:THR:CG2	2:H:300:GLU:H	2.18	0.56
2:D:248:ILE:CD1	2:D:355:ALA:HB3	2.36	0.56
2:D:288:LEU:HG	2:D:292:LEU:HD22	1.88	0.56
1:A:1:GLY:HA2	1:A:80:TYR:CD1	2.41	0.56
1:C:1:GLY:HA2	1:C:80:TYR:CD1	2.41	0.56
2:H:180:LEU:HG	2:H:184:MET:CE	2.36	0.56
2:B:180:LEU:HG	2:B:184:MET:CE	2.36	0.56
2:F:288:LEU:HG	2:F:292:LEU:HD22	1.88	0.56
2:F:346:THR:CG2	2:F:347:CYS:N	2.70	0.55
2:B:288:LEU:HG	2:B:292:LEU:HD22	1.88	0.55
2:H:288:LEU:HG	2:H:292:LEU:HD22	1.88	0.55
2:D:180:LEU:HG	2:D:184:MET:CE	2.36	0.55
1:E:1:GLY:HA2	1:E:80:TYR:CD1	2.41	0.55
1:A:4:VAL:HG22	1:A:74:LEU:HD22	1.87	0.55
2:F:313:LEU:HB3	2:F:404:MET:HE1	1.89	0.55
2:D:177:LEU:HD13	2:D:224:TRP:CZ3	2.42	0.55
2:F:331:HIS:HE1	2:F:350:ALA:O	1.90	0.55
2:H:346:THR:CG2	2:H:347:CYS:N	2.69	0.55
2:D:346:THR:CG2	2:D:347:CYS:N	2.70	0.54
2:F:443:LYS:HG2	2:F:448:GLN:NE2	2.17	0.54
2:B:346:THR:CG2	2:B:347:CYS:N	2.70	0.54
2:H:177:LEU:HD13	2:H:224:TRP:CZ3	2.42	0.54
2:B:331:HIS:HE1	2:B:350:ALA:O	1.90	0.54
2:B:177:LEU:HD13	2:B:224:TRP:CZ3	2.42	0.54
1:E:88:PRO:HB2	2:F:246:ALA:CB	2.37	0.54
1:E:85:THR:HG21	2:F:267:ASN:HD22	1.73	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:432:VAL:HG13	2:F:433:PRO:HD2	1.90	0.54
2:B:177:LEU:HD11	2:B:201:ILE:HD13	1.90	0.54
2:D:331:HIS:HE1	2:D:350:ALA:O	1.91	0.54
2:D:177:LEU:HD11	2:D:201:ILE:HD13	1.90	0.53
2:D:443:LYS:HG2	2:D:448:GLN:NE2	2.16	0.53
2:B:432:VAL:HG13	2:B:433:PRO:HD2	1.90	0.53
2:D:313:LEU:HB3	2:D:404:MET:HE1	1.90	0.53
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.90	0.53
2:F:177:LEU:HD13	2:F:224:TRP:CZ3	2.42	0.53
2:H:331:HIS:HE1	2:H:350:ALA:O	1.91	0.53
2:H:177:LEU:HD11	2:H:201:ILE:HD13	1.90	0.53
2:B:409:TRP:HB2	2:B:471:MET:HE3	1.91	0.53
2:H:248:ILE:HD12	2:H:355:ALA:HB3	1.91	0.53
2:D:180:LEU:HG	2:D:184:MET:HE2	1.89	0.53
2:F:201:ILE:O	2:F:205:ILE:HG13	2.09	0.53
2:F:177:LEU:HD11	2:F:201:ILE:HD13	1.90	0.52
2:F:258:ASN:C	2:F:348:CYS:HA	2.29	0.52
2:H:432:VAL:HG13	2:H:433:PRO:HD2	1.90	0.52
2:D:433:PRO:O	2:D:436:PRO:HG3	2.10	0.52
2:D:252:VAL:HG13	2:D:327:PRO:HD2	1.91	0.52
2:B:180:LEU:HG	2:B:184:MET:HE2	1.90	0.52
2:B:272:THR:HG1	2:B:273:TRP:HE3	1.58	0.52
1:E:16:PRO:HG2	1:E:64:ALA:HA	1.92	0.52
2:D:258:ASN:O	2:D:348:CYS:HA	2.09	0.52
2:B:288:LEU:HD21	2:B:411:ILE:HD11	1.92	0.52
2:F:433:PRO:O	2:F:436:PRO:HG3	2.09	0.52
2:H:201:ILE:O	2:H:205:ILE:HG13	2.09	0.52
2:F:409:TRP:HB2	2:F:471:MET:HE3	1.92	0.52
2:B:201:ILE:O	2:B:205:ILE:HG13	2.10	0.52
2:D:201:ILE:O	2:D:205:ILE:HG13	2.09	0.52
1:A:16:PRO:HG2	1:A:64:ALA:HA	1.91	0.52
2:B:433:PRO:O	2:B:436:PRO:HG3	2.10	0.52
2:F:272:THR:HG1	2:F:273:TRP:HE3	1.57	0.51
2:H:216:PHE:CE2	2:H:372:ARG:CD	2.85	0.51
1:G:16:PRO:HG2	1:G:64:ALA:HA	1.92	0.51
2:F:180:LEU:HG	2:F:184:MET:HE2	1.92	0.51
1:C:16:PRO:HG2	1:C:64:ALA:HA	1.91	0.51
2:B:244:ARG:NH1	2:B:368:ALA:HB2	2.26	0.51
2:D:193:LEU:HD11	2:D:201:ILE:HD12	1.92	0.51
2:D:253:MET:HE3	2:D:255:ARG:HD2	1.93	0.51
2:F:288:LEU:HD21	2:F:411:ILE:HD11	1.92	0.51



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:B:346:THR:HG22	2:B:347:CYS:N	2.26	0.51	
2:H:288:LEU:HD21	2:H:411:ILE:HD11	1.92	0.51	
2:D:288:LEU:HD21	2:D:411:ILE:HD11	1.91	0.51	
2:F:346:THR:HG22	2:F:347:CYS:N	2.26	0.51	
2:H:232:LYS:HD2	2:H:234:PHE:CE1	2.46	0.51	
2:F:248:ILE:CD1	2:F:355:ALA:HB3	2.41	0.50	
2:H:433:PRO:O	2:H:436:PRO:HG3	2.10	0.50	
1:A:42:ARG:HD2	2:B:184:MET:HG2	1.93	0.50	
2:D:346:THR:HG22	2:D:347:CYS:N	2.26	0.50	
2:H:253:MET:HE3	2:H:255:ARG:HD2	1.93	0.50	
2:D:283:HIS:CE1	2:D:342:LYS:HG2	2.46	0.50	
2:F:232:LYS:HD2	2:F:234:PHE:CE1	2.46	0.50	
2:H:193:LEU:HD11	2:H:201:ILE:HD12	1.92	0.50	
2:F:258:ASN:O	2:F:348:CYS:HA	2.12	0.50	
2:H:344:ASN:OD1	2:H:346:THR:HB	2.12	0.50	
2:D:232:LYS:HD2	2:D:234:PHE:CE1	2.46	0.50	
2:F:344:ASN:OD1	2:F:346:THR:HB	2.12	0.50	
2:D:248:ILE:HD12	2:D:355:ALA:HB3	1.94	0.50	
2:B:232:LYS:HD2	2:B:234:PHE:CE1	2.47	0.49	
1:E:88:PRO:HB2	2:F:246:ALA:HB3	1.94	0.49	
2:B:253:MET:HE3	2:B:255:ARG:HD2	1.94	0.49	
2:B:344:ASN:OD1	2:B:346:THR:HB	2.12	0.49	
2:D:272:THR:HG1	2:D:273:TRP:HE3	1.58	0.49	
2:F:432:VAL:CG1	2:F:436:PRO:HG3	2.43	0.49	
2:D:323:THR:C	2:D:325:GLY:H	2.15	0.49	
2:H:272:THR:HG1	2:H:273:TRP:HE3	1.59	0.49	
2:D:432:VAL:HG13	2:D:433:PRO:CD	2.43	0.49	
1:A:50:LEU:HD12	1:A:60:GLU:HG3	1.95	0.49	
2:D:344:ASN:OD1	2:D:346:THR:HB	2.12	0.49	
2:F:323:THR:C	2:F:325:GLY:H	2.15	0.49	
2:B:432:VAL:CG1	2:B:436:PRO:HG3	2.43	0.49	
2:B:323:THR:C	2:B:325:GLY:H	2.15	0.49	
1:C:88:PRO:HG3	2:D:243:PHE:CD1	2.48	0.49	
2:H:432:VAL:HG13	2:H:433:PRO:CD	2.43	0.48	
2:D:432:VAL:CG1	2:D:436:PRO:HG3	2.43	0.48	
2:F:471:MET:HE3	2:F:475:TRP:CH2	2.48	0.48	
2:H:346:THR:HG22	2:H:347:CYS:N	2.26	0.48	
2:B:432:VAL:HG13	2:B:433:PRO:CD	2.43	0.48	
1:C:50:LEU:HD12	1:C:60:GLU:HG3	1.95	0.48	
2:H:492:LEU:HD12	2:H:492:LEU:HA	1.73	0.48	
2:D:258:ASN:C	2:D:348:CYS:HA	2.34	0.48	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:F:362:THR:O	2:F:364:THR:HG23	2.14	0.48	
2:F:432:VAL:HG13	2:F:433:PRO:CD	2.43	0.48	
2:H:323:THR:C	2:H:325:GLY:H	2.15	0.48	
1:E:88:PRO:HB3	2:F:246:ALA:HB3	1.96	0.48	
2:B:362:THR:O	2:B:364:THR:HG23	2.14	0.48	
2:D:362:THR:O	2:D:364:THR:HG23	2.14	0.48	
2:H:432:VAL:CG1	2:H:436:PRO:HG3	2.43	0.48	
1:E:50:LEU:HD12	1:E:60:GLU:HG3	1.95	0.48	
2:B:389:ASN:ND2	2:B:391:LYS:H	2.12	0.47	
1:C:90:ILE:HG13	2:D:250:GLN:HG2	1.94	0.47	
2:F:450:LEU:O	2:F:451:ARG:HD3	2.14	0.47	
2:B:297:VAL:HG22	2:B:298:THR:N	2.30	0.47	
2:B:471:MET:HE3	2:B:475:TRP:CH2	2.49	0.47	
2:F:389:ASN:ND2	2:F:391:LYS:H	2.12	0.47	
1:G:50:LEU:HD12	1:G:60:GLU:HG3	1.95	0.47	
2:D:389:ASN:ND2	2:D:391:LYS:H	2.13	0.47	
2:F:253:MET:HE3	2:F:255:ARG:HD2	1.96	0.47	
2:B:193:LEU:HD11	2:B:201:ILE:HD12	1.92	0.47	
2:B:450:LEU:O	2:B:451:ARG:HD3	2.15	0.47	
2:H:297:VAL:HG22	2:H:298:THR:N	2.30	0.47	
2:D:450:LEU:O	2:D:451:ARG:HD3	2.14	0.47	
2:F:363:ASP:OD1	2:F:363:ASP:O	2.33	0.47	
2:H:362:THR:O	2:H:364:THR:HG23	2.14	0.47	
2:B:363:ASP:OD1	2:B:363:ASP:O	2.33	0.47	
2:F:208:GLN:C	2:F:209:GLU:HG3	2.35	0.47	
2:F:297:VAL:HG22	2:F:298:THR:N	2.30	0.47	
2:H:208:GLN:C	2:H:209:GLU:HG3	2.35	0.47	
2:D:184:MET:CE	2:D:193:LEU:HD22	2.45	0.47	
2:D:260:LEU:HD13	2:D:340:LEU:HD12	1.97	0.47	
2:D:270:ASN:C	2:D:272:THR:H	2.18	0.47	
2:F:193:LEU:HD11	2:F:201:ILE:HD12	1.92	0.47	
1:G:26:TYR:HA	1:G:100:ASP:O	2.15	0.47	
2:D:297:VAL:HG22	2:D:298:THR:N	2.30	0.47	
2:F:252:VAL:HG11	2:F:329:ILE:CD1	2.42	0.47	
2:B:432:VAL:HG12	2:B:433:PRO:O	2.15	0.46	
2:F:432:VAL:HG12	2:F:433:PRO:O	2.15	0.46	
2:B:484:THR:HG23	2:B:486:LEU:H	1.80	0.46	
2:H:389:ASN:ND2	2:H:391:LYS:H	2.12	0.46	
2:H:450:LEU:O	2:H:451:ARG:HD3	2.15	0.46	
1:A:91:ILE:HA	1:A:92:PRO:HD3	1.83	0.46	
1:C:26:TYR:CZ	2:D:196:LEU:HD22	2.50	0.46	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:208:GLN:C	2:D:209:GLU:HG3	2.35	0.46
2:F:492:LEU:HD12	2:F:492:LEU:HA	1.73	0.46
2:D:484:THR:HG23	2:D:486:LEU:H	1.80	0.46
1:G:8:SER:HA	1:G:9:PRO:HD3	1.80	0.46
2:H:184:MET:CE	2:H:193:LEU:HD22	2.45	0.46
2:H:363:ASP:OD1	2:H:363:ASP:O	2.33	0.46
2:H:432:VAL:HG12	2:H:433:PRO:O	2.16	0.46
2:D:413:ARG:NH1	2:D:422:GLU:HB3	2.31	0.46
2:D:492:LEU:HD12	2:D:492:LEU:HA	1.73	0.46
1:E:26:TYR:HA	1:E:100:ASP:O	2.15	0.46
1:E:90:ILE:HG12	2:F:250:GLN:HG2	1.97	0.46
2:B:413:ARG:NH1	2:B:422:GLU:HB3	2.31	0.46
2:F:409:TRP:HD1	2:F:471:MET:CE	2.27	0.46
2:F:484:THR:HG23	2:F:486:LEU:H	1.80	0.46
2:H:413:ARG:NH1	2:H:422:GLU:HB3	2.31	0.46
2:D:363:ASP:OD1	2:D:363:ASP:O	2.33	0.46
2:D:432:VAL:HG12	2:D:433:PRO:O	2.16	0.46
2:F:270:ASN:C	2:F:272:THR:H	2.18	0.46
2:H:244:ARG:HG2	2:H:368:ALA:CB	2.46	0.46
2:H:373:VAL:HG22	2:H:374:GLY:H	1.81	0.46
2:B:270:ASN:C	2:B:272:THR:H	2.18	0.45
2:B:357:ARG:HD2	2:B:359:ASP:OD1	2.17	0.45
1:C:26:TYR:HA	1:C:100:ASP:O	2.16	0.45
1:A:26:TYR:HA	1:A:100:ASP:O	2.16	0.45
2:F:258:ASN:ND2	2:F:308:SER:HB2	2.31	0.45
2:H:270:ASN:C	2:H:272:THR:H	2.18	0.45
2:B:235:SER:H	2:B:235:SER:HG	1.60	0.45
2:D:410:GLU:OE1	2:D:424:TYR:OH	2.27	0.45
2:F:413:ARG:NH1	2:F:422:GLU:HB3	2.31	0.45
2:H:357:ARG:HD2	2:H:359:ASP:OD1	2.16	0.45
2:H:484:THR:HG23	2:H:486:LEU:H	1.80	0.45
2:D:381:PRO:HD2	2:D:382:GLU:OE2	2.17	0.45
2:D:471:MET:HE3	2:D:475:TRP:CH2	2.52	0.45
2:D:294:ARG:HD2	2:D:295:TYR:CE1	2.52	0.45
2:H:294:ARG:HD2	2:H:295:TYR:CE1	2.52	0.45
2:B:373:VAL:HG22	2:B:374:GLY:H	1.81	0.45
2:B:381:PRO:HD2	2:B:382:GLU:OE2	2.17	0.45
2:D:216:PHE:CZ	2:D:372:ARG:HD2	2.52	0.45
2:D:331:HIS:O	2:D:332:ARG:HB2	2.17	0.45
2:F:373:VAL:HG22	2:F:374:GLY:H	1.81	0.45
2:H:331:HIS:O	2:H:332:ARG:HB2	2.17	0.45



	io ao pagoini	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:D:406:LEU:HB3	2:D:427:PRO:HG2	1.99	0.45	
1:E:90:ILE:HG12	2:F:250:GLN:CG	2.46	0.45	
2:F:381:PRO:HD2	2:F:382:GLU:OE2	2.17	0.45	
1:A:17:LYS:N	1:A:20:GLN:OE1	2.49	0.45	
2:B:294:ARG:HD2	2:B:295:TYR:CE1	2.52	0.45	
2:B:484:THR:HG22	2:B:487:ARG:N	2.12	0.45	
1:C:85:THR:HG21	2:D:267:ASN:HD22	1.81	0.45	
2:F:294:ARG:HD2	2:F:295:TYR:CE1	2.52	0.45	
2:H:381:PRO:HD2	2:H:382:GLU:OE2	2.17	0.45	
2:F:336:SER:OG	2:F:410:GLU:CD	2.56	0.45	
2:D:373:VAL:HG22	2:D:374:GLY:H	1.82	0.44	
2:F:216:PHE:HD2	2:F:238:GLU:CG	2.28	0.44	
2:D:357:ARG:HD2	2:D:359:ASP:OD1	2.16	0.44	
2:D:484:THR:HG22	2:D:487:ARG:N	2.13	0.44	
1:C:17:LYS:N	1:C:20:GLN:OE1	2.49	0.44	
2:H:368:ALA:HA	2:H:369:PRO:HD3	1.68	0.44	
2:H:432:VAL:HG11	2:H:436:PRO:CG	2.48	0.44	
1:A:1:GLY:HA2	1:A:80:TYR:CG	2.52	0.44	
2:B:336:SER:OG	2:B:410:GLU:CD	2.56	0.44	
2:D:435:ASP:N	2:D:436:PRO:HD3	2.32	0.44	
2:F:406:LEU:HB3	2:F:427:PRO:HG2	2.00	0.44	
2:H:216:PHE:HD2	2:H:238:GLU:CG	2.28	0.44	
2:B:208:GLN:C	2:B:209:GLU:HG3	2.35	0.44	
2:F:184:MET:CE	2:F:193:LEU:HD22	2.46	0.44	
2:F:357:ARG:HD2	2:F:359:ASP:OD1	2.17	0.44	
2:F:432:VAL:HG11	2:F:436:PRO:CG	2.47	0.44	
1:A:84:ALA:O	1:A:93:PRO:CB	2.66	0.44	
2:B:435:ASP:N	2:B:436:PRO:HD3	2.32	0.44	
1:C:1:GLY:HA2	1:C:80:TYR:CG	2.53	0.44	
1:C:84:ALA:O	1:C:93:PRO:CB	2.66	0.44	
1:G:1:GLY:HA2	1:G:80:TYR:CG	2.52	0.44	
2:B:331:HIS:O	2:B:332:ARG:HB2	2.17	0.44	
2:D:177:LEU:O	2:D:181:ILE:HG13	2.18	0.44	
2:D:203:ARG:NH1	2:D:268:LYS:HG3	2.33	0.44	
2:F:331:HIS:O	2:F:332:ARG:HB2	2.17	0.44	
2:B:406:LEU:HB3	2:B:427:PRO:HG2	2.00	0.44	
2:B:409:TRP:HD1	2:B:471:MET:CE	2.27	0.44	
2:D:177:LEU:HD13	2:D:224:TRP:CE3	2.53	0.44	
1:E:84:ALA:O	1:E:93:PRO:CB	2.66	0.44	
2:H:252:VAL:HG11	2:H:329:ILE:HD11	1.99	0.44	
2:H:435:ASP:N	2:H:436:PRO:HD3	2.33	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:B:177:LEU:O	2:B:181:ILE:HG13	2.18	0.44	
2:B:278:LEU:HD12	2:B:278:LEU:HA	1.87	0.44	
2:D:335:LYS:HD3	2:D:337:LYS:HB2	2.00	0.44	
2:D:432:VAL:HG11	2:D:436:PRO:CG	2.48	0.44	
2:F:177:LEU:O	2:F:181:ILE:HG13	2.18	0.44	
2:H:216:PHE:HE2	2:H:372:ARG:HD2	1.74	0.44	
2:B:203:ARG:NH1	2:B:268:LYS:HG3	2.33	0.43	
2:B:321:VAL:HG12	2:B:322:GLY:N	2.33	0.43	
2:B:335:LYS:HD3	2:B:337:LYS:HB2	2.00	0.43	
2:D:235:SER:HG	2:D:238:GLU:CD	2.22	0.43	
2:F:335:LYS:HD3	2:F:337:LYS:HB2	2.00	0.43	
1:G:84:ALA:O	1:G:93:PRO:CB	2.66	0.43	
2:H:406:LEU:HB3	2:H:427:PRO:HG2	2.00	0.43	
2:B:216:PHE:HD2	2:B:238:GLU:CG	2.28	0.43	
2:D:321:VAL:HG12	2:D:322:GLY:N	2.33	0.43	
2:F:203:ARG:NH1	2:F:268:LYS:HG3	2.33	0.43	
1:E:1:GLY:HA2	1:E:80:TYR:CG	2.53	0.43	
2:B:186:THR:O	2:B:187:SER:C	2.57	0.43	
2:H:177:LEU:HD13	2:H:224:TRP:CE3	2.53	0.43	
2:B:177:LEU:HD13	2:B:224:TRP:CE3	2.53	0.43	
2:B:432:VAL:HG11	2:B:436:PRO:CG	2.48	0.43	
2:F:235:SER:HG	2:F:238:GLU:CD	2.21	0.43	
2:F:385:ASP:C	2:F:385:ASP:OD1	2.57	0.43	
2:F:484:THR:HG22	2:F:487:ARG:N	2.13	0.43	
2:H:331:HIS:HD2	2:H:333:ASP:N	2.12	0.43	
2:D:186:THR:O	2:D:187:SER:C	2.57	0.43	
2:B:398:ARG:HD3	2:B:479:GLY:C	2.39	0.43	
2:D:398:ARG:HD3	2:D:479:GLY:C	2.39	0.43	
2:F:177:LEU:HD13	2:F:224:TRP:CE3	2.53	0.43	
2:F:389:ASN:C	2:F:389:ASN:HD22	2.22	0.43	
2:H:385:ASP:C	2:H:385:ASP:OD1	2.57	0.43	
1:C:8:SER:HA	1:C:9:PRO:HD3	1.81	0.43	
2:D:336:SER:OG	2:D:410:GLU:CD	2.56	0.43	
1:E:87:HIS:HE1	2:F:265:ALA:O	2.02	0.43	
2:F:435:ASP:N	2:F:436:PRO:HD3	2.32	0.43	
2:H:177:LEU:O	2:H:181:ILE:HG13	2.18	0.43	
2:B:391:LYS:O	2:B:391:LYS:HG2	2.19	0.43	
2:H:203:ARG:NH1	2:H:268:LYS:HG3	2.33	0.43	
2:D:391:LYS:O	2:D:391:LYS:HG2	2.19	0.43	
1:E:17:LYS:N	1:E:20:GLN:OE1	2.49	0.43	
2:F:432:VAL:CG1	2:F:436:PRO:CG	2.97	0.43	



	lo ao pagom	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:E:91:ILE:HA	1:E:92:PRO:HD3	1.83	0.42	
2:H:336:SER:OG	2:H:410:GLU:CD	2.57	0.42	
2:H:389:ASN:C	2:H:389:ASN:HD22	2.23	0.42	
2:H:391:LYS:O	2:H:391:LYS:HG2	2.19	0.42	
2:B:252:VAL:HG11	2:B:329:ILE:CD1	2.46	0.42	
2:B:487:ARG:O	2:B:491:THR:HG23	2.19	0.42	
2:H:321:VAL:HG12	2:H:322:GLY:N	2.33	0.42	
2:H:335:LYS:HD3	2:H:337:LYS:HB2	2.00	0.42	
2:B:368:ALA:HA	2:B:369:PRO:HD3	1.68	0.42	
2:H:330:ALA:HB3	2:H:356:VAL:HG22	2.01	0.42	
1:C:91:ILE:HA	1:C:92:PRO:HD3	1.83	0.42	
2:D:385:ASP:OD1	2:D:385:ASP:C	2.57	0.42	
2:F:180:LEU:HG	2:F:184:MET:HE1	2.01	0.42	
2:F:391:LYS:HG2	2:F:391:LYS:O	2.19	0.42	
2:F:398:ARG:HD3	2:F:479:GLY:C	2.39	0.42	
2:B:184:MET:CE	2:B:193:LEU:HD22	2.45	0.42	
2:B:244:ARG:HG2	2:B:368:ALA:CB	2.49	0.42	
2:D:432:VAL:CG1	2:D:436:PRO:CG	2.97	0.42	
1:E:90:ILE:HD11	2:F:250:GLN:OE1	2.20	0.42	
2:H:398:ARG:HD3	2:H:479:GLY:C	2.39	0.42	
2:B:330:ALA:HB3	2:B:356:VAL:HG22	2.02	0.42	
2:B:389:ASN:HD22	2:B:389:ASN:C	2.22	0.42	
2:B:385:ASP:OD1	2:B:385:ASP:C	2.57	0.42	
2:D:331:HIS:HD2	2:D:333:ASP:N	2.12	0.42	
2:F:321:VAL:HG12	2:F:322:GLY:N	2.33	0.42	
2:F:330:ALA:HB3	2:F:356:VAL:HG22	2.02	0.42	
2:H:235:SER:H	2:H:235:SER:HG	1.60	0.42	
1:C:71:ARG:HA	1:C:101:VAL:O	2.20	0.42	
2:D:216:PHE:HD2	2:D:238:GLU:CG	2.28	0.42	
2:D:389:ASN:C	2:D:389:ASN:HD22	2.22	0.42	
1:E:88:PRO:HB2	2:F:246:ALA:HB1	2.02	0.42	
2:F:186:THR:O	2:F:187:SER:C	2.57	0.42	
1:G:105:LYS:HE3	1:G:107:GLU:OE2	2.20	0.42	
2:H:487:ARG:O	2:H:491:THR:HG23	2.20	0.42	
1:A:105:LYS:HE3	1:A:107:GLU:OE2	2.20	0.42	
2:B:177:LEU:HD12	2:B:177:LEU:HA	1.87	0.42	
2:D:330:ALA:HB3	2:D:356:VAL:HG22	2.01	0.42	
2:D:487:ARG:O	2:D:491:THR:HG23	2.19	0.42	
1:G:71:ARG:HA	1:G:101:VAL:O	2.20	0.42	
2:H:238:GLU:O	2:H:239:GLU:C	2.58	0.42	
2:H:432:VAL:CG1	2:H:436:PRO:CG	2.97	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:H:489:LYS:HD2	2:H:489:LYS:C	2.41	0.42	
1:A:90:ILE:HG13	2:B:250:GLN:HG2	2.02	0.42	
2:B:432:VAL:CG1	2:B:436:PRO:CG	2.97	0.42	
2:F:177:LEU:HD12	2:F:177:LEU:HA	1.87	0.42	
1:A:71:ARG:HA	1:A:101:VAL:O	2.20	0.41	
2:F:489:LYS:HD2	2:F:489:LYS:C	2.41	0.41	
2:H:186:THR:O	2:H:187:SER:C	2.57	0.41	
2:B:248:ILE:HD13	2:B:355:ALA:HB3	1.97	0.41	
2:F:487:ARG:O	2:F:491:THR:HG23	2.19	0.41	
2:B:238:GLU:O	2:B:239:GLU:C	2.59	0.41	
2:B:285:HIS:HB2	2:B:341:VAL:O	2.20	0.41	
2:D:186:THR:HG22	2:D:187:SER:N	2.36	0.41	
2:H:252:VAL:HG13	2:H:327:PRO:HD2	2.02	0.41	
2:H:471:MET:HE3	2:H:475:TRP:CH2	2.55	0.41	
2:B:489:LYS:C	2:B:489:LYS:HD2	2.41	0.41	
2:D:285:HIS:HB2	2:D:341:VAL:O	2.20	0.41	
2:D:445:VAL:HG13	2:D:451:ARG:NH1	2.36	0.41	
2:B:270:ASN:C	2:B:272:THR:N	2.74	0.41	
2:F:204:THR:O	2:F:204:THR:CG2	2.69	0.41	
1:G:26:TYR:CZ	2:H:196:LEU:HD22	2.56	0.41	
2:B:410:GLU:OE1	2:B:424:TYR:OH	2.26	0.41	
1:C:105:LYS:HE3	1:C:107:GLU:OE2	2.20	0.41	
2:D:254:LEU:HD21	2:D:326:LYS:HE2	2.02	0.41	
2:D:334:LEU:HD23	2:D:334:LEU:HA	1.90	0.41	
2:F:180:LEU:HD12	2:F:180:LEU:HA	1.96	0.41	
2:H:285:HIS:HB2	2:H:341:VAL:O	2.21	0.41	
2:B:186:THR:HG22	2:B:187:SER:N	2.35	0.41	
2:D:287:SER:HA	2:D:339:ILE:O	2.21	0.41	
1:C:90:ILE:CG1	2:D:250:GLN:HG2	2.50	0.41	
2:F:216:PHE:HB3	2:F:238:GLU:HG2	2.03	0.41	
2:B:216:PHE:HB3	2:B:238:GLU:HG2	2.03	0.41	
2:B:445:VAL:HG13	2:B:451:ARG:NH1	2.35	0.41	
1:E:71:ARG:HA	1:E:101:VAL:O	2.20	0.41	
2:F:270:ASN:C	2:F:272:THR:N	2.74	0.41	
2:F:331:HIS:HD2	2:F:333:ASP:N	2.12	0.41	
2:H:270:ASN:C	2:H:272:THR:N	2.74	0.41	
2:H:388:ILE:HG23	2:H:388:ILE:O	2.21	0.41	
2:H:445:VAL:HG13	2:H:451:ARG:NH1	2.35	0.41	
1:A:87:HIS:HA	1:A:88:PRO:HD3	1.93	0.41	
2:B:287:SER:HA	2:B:339:ILE:O	2.21	0.41	
2:D:270:ASN:C	2:D:272:THR:N	2.74	0.41	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:287:SER:HA	2:F:339:ILE:O	2.21	0.41
2:F:289:PHE:HB2	2:F:336:SER:HB2	2.03	0.41
2:B:238:GLU:HB3	2:B:241:SER:HB2	2.03	0.40
2:B:289:PHE:HB2	2:B:336:SER:HB2	2.03	0.40
2:D:272:THR:OG1	2:D:273:TRP:HE3	2.04	0.40
2:D:298:THR:CG2	2:D:299:VAL:N	2.84	0.40
1:E:105:LYS:HE3	1:E:107:GLU:OE2	2.20	0.40
1:G:91:ILE:HA	1:G:92:PRO:HD3	1.83	0.40
2:B:272:THR:OG1	2:B:273:TRP:HE3	2.04	0.40
2:F:285:HIS:HB2	2:F:341:VAL:O	2.20	0.40
2:F:445:VAL:HG13	2:F:451:ARG:NH1	2.36	0.40
1:G:17:LYS:N	1:G:20:GLN:OE1	2.49	0.40
2:B:258:ASN:O	2:B:348:CYS:HA	2.21	0.40
2:B:298:THR:CG2	2:B:299:VAL:N	2.84	0.40
2:D:289:PHE:HB2	2:D:336:SER:HB2	2.03	0.40
2:D:388:ILE:O	2:D:388:ILE:HG23	2.21	0.40
2:D:489:LYS:C	2:D:489:LYS:HD2	2.41	0.40
2:H:186:THR:HG22	2:H:187:SER:N	2.36	0.40
2:H:272:THR:OG1	2:H:273:TRP:HE3	2.04	0.40
2:D:184:MET:HE3	2:D:193:LEU:CD2	2.50	0.40
2:F:258:ASN:O	2:F:349:ILE:N	2.45	0.40
2:H:238:GLU:HB3	2:H:241:SER:HB2	2.03	0.40
2:H:258:ASN:O	2:H:348:CYS:HA	2.22	0.40
2:H:287:SER:HA	2:H:339:ILE:O	2.21	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	Percen	ntiles
1	А	105/107~(98%)	99~(94%)	6~(6%)	0	100	100



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	С	105/107~(98%)	99~(94%)	6~(6%)	0	100	100
1	Е	105/107~(98%)	99~(94%)	6 (6%)	0	100	100
1	G	105/107~(98%)	99~(94%)	6 (6%)	0	100	100
2	В	324/342~(95%)	306 (94%)	18 (6%)	0	100	100
2	D	324/342~(95%)	307~(95%)	17 (5%)	0	100	100
2	F	324/342~(95%)	306 (94%)	18 (6%)	0	100	100
2	Н	324/342~(95%)	307~(95%)	17 (5%)	0	100	100
All	All	1716/1796~(96%)	1622 (94%)	94 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	89/89~(100%)	87~(98%)	2(2%)	52 76
1	С	89/89~(100%)	87~(98%)	2(2%)	52 76
1	Ε	89/89~(100%)	87~(98%)	2(2%)	52 76
1	G	89/89~(100%)	87~(98%)	2(2%)	52 76
2	В	279/294~(95%)	261 (94%)	18 (6%)	17 34
2	D	279/294~(95%)	261 (94%)	18 (6%)	17 34
2	F	279/294~(95%)	261 (94%)	18 (6%)	17 34
2	Н	279/294~(95%)	261 (94%)	18 (6%)	17 34
All	All	1472/1532~(96%)	1392 (95%)	80 (5%)	22 44

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	25	HIS
1	А	59	TRP



Mol	Chain	Res	Type
2	В	177	LEU
2	В	209	GLU
2	В	244	ARG
2	В	273	TRP
2	В	292	LEU
2	В	294	ARG
2	В	298	THR
2	В	307	LEU
2	В	335	LYS
2	В	341	VAL
2	В	389	ASN
2	В	422	GLU
2	В	484	THR
2	В	486	LEU
2	В	487	ARG
2	В	489	LYS
2	В	491	THR
2	В	492	LEU
1	С	25	HIS
1	С	59	TRP
2	D	177	LEU
2	D	209	GLU
2	D	244	ARG
2	D	273	TRP
2	D	292	LEU
2	D	294	ARG
2	D	298	THR
2	D	307	LEU
2	D	335	LYS
2	D	341	VAL
2	D	389	ASN
2	D	422	GLU
2	D	484	THR
2	D	486	LEU
2	D	487	ARG
2	D	489	LYS
2	D	491	THR
2	D	492	LEU
1	Е	25	HIS
1	Е	59	TRP
2	F	177	LEU
2	F	209	GLU



Mol	Chain	Res	Type
2	F	244	ARG
2	F	273	TRP
2	F	292	LEU
2	F	294	ARG
2	F	298	THR
2	F	307	LEU
2	F	335	LYS
2	F	341	VAL
2	F	389	ASN
2	F	422	GLU
2	F	484	THR
2	F	486	LEU
2	F	487	ARG
2	F	489	LYS
2	F	491	THR
2	F	492	LEU
1	G	25	HIS
1	G	59	TRP
2	Н	177	LEU
2	Н	209	GLU
2	Н	244	ARG
2	Н	273	TRP
2	Н	292	LEU
2	Н	294	ARG
2	Н	298	THR
2	Н	307	LEU
2	Н	335	LYS
2	Н	341	VAL
2	Н	389	ASN
2	Н	422	GLU
2	Н	484	THR
2	Н	486	LEU
2	Н	487	ARG
2	Н	489	LYS
2	Н	491	THR
2	Н	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	В	256	HIS
2	В	315	HIS



Mol	Chain	Res	Type
2	В	331	HIS
2	В	389	ASN
2	В	448	GLN
2	В	494	GLN
1	С	87	HIS
2	D	256	HIS
2	D	258	ASN
2	D	331	HIS
2	D	389	ASN
2	D	448	GLN
2	D	494	GLN
1	Е	87	HIS
2	F	256	HIS
2	F	267	ASN
2	F	315	HIS
2	F	331	HIS
2	F	389	ASN
2	F	448	GLN
2	F	494	GLN
2	Н	256	HIS
2	Н	331	HIS
2	Н	389	ASN
2	Н	448	GLN
2	Н	494	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.



1B6C

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 Chair		Chain	Dec	Tinle	Bond lengths			Bond angles		
IVIOI	Type	Chain	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	SO4	В	158	-	4,4,4	0.42	0	$6,\!6,\!6$	0.18	0
3	SO4	Н	504	-	4,4,4	0.43	0	$6,\!6,\!6$	0.18	0
3	SO4	F	504	-	4,4,4	0.46	0	$6,\!6,\!6$	0.18	0
3	SO4	D	504	-	4,4,4	0.46	0	$6,\!6,\!6$	0.19	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	158	SO4	1	0
3	Н	504	SO4	1	0
3	F	504	SO4	1	0
3	D	504	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:



Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	283:HIS	С	284:GLU	Ν	1.19



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	107/107~(100%)	-0.02	0 100 100	31, 40, 51, 57	2(1%)
1	С	107/107~(100%)	0.08	3 (2%) 53 46	31, 40, 52, 58	2(1%)
1	E	107/107~(100%)	0.14	2 (1%) 66 62	32, 41, 52, 58	2(1%)
1	G	107/107~(100%)	0.03	1 (0%) 84 82	31, 40, 51, 57	2(1%)
2	В	326/342~(95%)	0.05	10 (3%) 49 42	13, 31, 66, 85	5(1%)
2	D	326/342~(95%)	0.18	18 (5%) 25 19	15, 32, 66, 86	5(1%)
2	F	326/342~(95%)	0.48	31 (9%) 8 5	16, 33, 66, 86	5(1%)
2	Н	326/342~(95%)	0.08	12 (3%) 41 34	15, 31, 66, 86	5 (1%)
All	All	1732/1796~(96%)	0.16	77 (4%) 34 27	13, 36, 60, 86	28 (1%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	270	ASN	7.9
2	D	272	THR	7.8
2	Н	271	GLY	7.7
2	F	371	HIS	7.3
2	D	324	GLN	7.2
2	F	271	GLY	7.1
2	F	324	GLN	6.5
2	F	272	THR	6.2
2	Н	272	THR	6.2
2	F	322	GLY	6.1
2	F	321	VAL	6.1
2	F	269	ASP	6.0
2	В	272	THR	5.9
2	В	271	GLY	5.3
2	F	273	TRP	5.3
2	F	369	PRO	5.3



Mol	Chain	Res	Type	RSRZ
2	F	323	THR	5.2
2	F	237	ARG	4.9
2	F	361	ALA	4.8
2	D	273	TRP	4.8
2	F	216	PHE	4.6
2	D	323	THR	4.5
2	D	325	GLY	4.4
2	D	494	GLN	4.2
2	D	271	GLY	4.2
2	D	270	ASN	4.0
2	F	372	ARG	4.0
2	Н	213	LYS	4.0
2	D	320	ILE	4.0
2	F	368	ALA	3.9
2	В	214	GLY	3.8
2	F	370	ASN	3.8
2	В	273	TRP	3.6
2	В	215	ARG	3.6
2	В	270	ASN	3.5
2	F	320	ILE	3.4
2	F	235	SER	3.4
2	D	321	VAL	3.3
2	F	238	GLU	3.2
2	Н	270	ASN	3.2
2	F	215	ARG	3.1
2	Н	273	TRP	3.1
2	F	325	GLY	3.1
2	D	237	ARG	3.1
2	F	359	ASP	2.9
2	D	215	ARG	2.9
2	D	359	ASP	2.8
2	F	494	GLN	2.8
2	F	244	ARG	2.7
2	D	361	ALA	2.7
2	В	499	GLU	2.7
2	D	362	THR	2.6
2	F	434	SER	2.6
2	D	211	ILE	2.5
2	F	362	THR	2.5
2	Н	362	THR	2.5
2	В	175	THR	2.4
2	Н	499	GLU	2.4



Mol	Chain	Res	Type	RSRZ
2	Н	175	THR	2.4
2	Н	237	ARG	2.4
2	F	499	GLU	2.4
2	Н	238	GLU	2.3
1	С	18	ARG	2.3
1	Е	1	GLY	2.3
2	F	375	THR	2.3
2	F	392	HIS	2.3
1	С	34	LYS	2.3
2	В	213	LYS	2.2
2	В	418	GLY	2.2
2	D	213	LYS	2.2
2	F	211	ILE	2.1
2	Н	361	ALA	2.1
1	Е	34	LYS	2.1
1	С	32	ASP	2.1
2	D	392	HIS	2.1
2	Н	418	GLY	2.1
1	G	18	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
3	SO4	F	504	5/5	0.58	0.56	$64,\!64,\!65,\!66$	0
3	SO4	D	504	5/5	0.65	0.37	63,64,64,65	0
3	SO4	Н	504	5/5	0.90	0.16	62,62,62,63	0
3	SO4	В	158	5/5	0.91	0.16	61,61,62,62	0



6.5 Other polymers (i)

There are no such residues in this entry.

