

Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 07:37 AM EDT

PDB ID	:	4HHM
Title	:	Crystal structure of a mutant, G219A, of Glucose Isomerase from Streptomyces
		sp. SK
Authors	:	Ben Hlima, H.; Riguet, J.; Haser, R.; Aghajari, N.
Deposited on	:	2012-10-10
Resolution	:	2.15 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
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
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)	:	2.35.1

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 2.15 Å.

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



Motria	Whole archive	Similar resolution		
	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1479 (2.16-2.16)		
Clashscore	141614	1585 (2.16-2.16)		
Ramachandran outliers	138981	1560 (2.16-2.16)		
Sidechain outliers	138945	1559 (2.16-2.16)		
RSRZ outliers	127900	1456 (2.16-2.16)		

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	388	80%	19%	
				10,0	
1	В	388	79%	20%	•
1	С	388	81%	18%	
1	D	388	77%	22%	•
1	Е	388	80%	19%	



Mol	Chain	Length	Quality of chain		
1	F	388	80%	19%	·
1	G	388	78%	21%	·
1	Н	388	80%	19%	·



4HHM

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26557 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					AltConf	Trace
1	Δ	286	Total	С	Ν	0	S	0	0	0
	A	300	3023	1911	540	564	8	0	0	0
1	В	386	Total	С	Ν	0	S	0	0	0
		300	3023	1911	540	564	8	0	0	0
1	С	386	Total	С	Ν	0	S	0	0	0
		500	3023	1911	540	564	8	0	0	0
1	D	386	Total	С	Ν	0	S	0	0	0
	D	360	3023	1911	540	564	8		0	0
1	F	386	Total	С	Ν	0	S	0	0	0
	Ľ	500	3023	1911	540	564	8		0	U
1	F	386	Total	С	Ν	0	\mathbf{S}	0	0	0
	I.	380	3023	1911	540	564	8	0	0	0
1	C	286	Total	С	Ν	0	S	0	0	0
I G	300	3023	1911	540	564	8	0	0	0	
1	ц	296	Total	С	Ν	0	S	0	0	0
		500	3023	1911	540	564	8		0	

• Molecule 1 is a protein called Xylose isomerase.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
В	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
С	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
D	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
Е	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
F	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
G	219	ALA	GLY	engineered mutation	UNP Q9ZAI3
Н	219	ALA	GLY	engineered mutation	UNP Q9ZAI3

• Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).



4HHM

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Co 1 1	0	0
2	В	1	Total Co 1 1	0	0
2	С	1	Total Co 1 1	0	0
2	D	1	Total Co 1 1	0	0
2	Е	1	Total Co 1 1	0	0
2	F	1	Total Co 1 1	0	0
2	G	1	Total Co 1 1	0	0
2	Н	1	Total Co 1 1	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	Е	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	Н	1	Total Mg 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	267	Total O 267 267	0	0
4	В	311	Total O 311 311	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	298	Total O 298 298	0	0
4	D	303	Total O 303 303	0	0
4	Е	308	Total O 308 308	0	0
4	F	276	Total O 276 276	0	0
4	G	293	Total O 293 293	0	0
4	Н	301	Total O 301 301	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: Xylose isomerase





• Molecule 1: Xylose isomerase



N300 D101 C306 A106 T312 A106 T312 R105 R36 R107 D336 T121 D344 R117 D345 R121 A343 R121 A344 Y134 A345 R121 A345 R121 A345 P182 A345 P182 A365 P182 A37 P182 A36 P182 A36 P182 A37 P182 P182 P182 P182 P182 P182 P182 P182 P182 P182

• Molecule 1: Xylose isomerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	85.50Å 137.40Å 136.60Å	Deperitor
a, b, c, α , β , γ	90.00° 90.06° 90.00°	Depositor
$\mathbf{P}_{\text{accolution}}\left(\overset{}{\boldsymbol{\lambda}}\right)$	48.50 - 2.15	Depositor
Resolution (A)	48.44 - 2.15	EDS
% Data completeness	(Not available) $(48.50-2.15)$	Depositor
(in resolution range)	95.3(48.44-2.15)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	0.07	Depositor
$< I/\sigma(I) > 1$	$2.79 (at 2.16 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
B B.	0.197 , 0.250	Depositor
Π, Π_{free}	0.201 , 0.255	DCC
R_{free} test set	8172 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	20.6	Xtriage
Anisotropy	0.851	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 17.3	EDS
L-test for twinning ²	$< L > = 0.45, < L^2 > = 0.28$	Xtriage
	0.030 for -h,-l,-k	
Estimated twinning fraction	0.034 for -h,l,k	Xtriage
	0.266 for h,-k,-l	
F_o, F_c correlation	0.95	EDS
Total number of atoms	26557	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.84% 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: CO, MG

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).

Mol Chain		Bond	lengths	Bond	angles
	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.39	0/3096	0.57	0/4202
1	В	0.39	0/3096	0.58	0/4202
1	С	0.36	0/3096	0.57	0/4202
1	D	0.38	0/3096	0.57	0/4202
1	Ε	0.38	0/3096	0.58	0/4202
1	F	0.35	0/3096	0.54	0/4202
1	G	0.40	0/3096	0.58	0/4202
1	Н	0.38	0/3096	0.59	0/4202
All	All	0.38	0/24768	0.57	0/33616

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	3023	0	2915	60	0
1	В	3023	0	2915	59	0
1	С	3023	0	2915	59	0
1	D	3023	0	2915	76	0
1	Е	3023	0	2915	59	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3023	0	2915	55	0
1	G	3023	0	2915	71	0
1	Н	3023	0	2915	58	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	Н	1	0	0	0	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
3	Е	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	Н	1	0	0	0	0
4	А	267	0	0	6	0
4	В	311	0	0	10	0
4	С	298	0	0	6	0
4	D	303	0	0	4	0
4	Е	308	0	0	5	0
4	F	276	0	0	2	0
4	G	293	0	0	5	0
4	Н	301	0	0	7	0
All	All	26557	0	23320	429	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 9.

All (429) 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 (\AA)	overlap (Å)
1:G:365:ALA:HA	1:G:368:ARG:HD2	1.52	0.92
1:F:24:ASP:HB2	1:F:25:PRO:HD2	1.54	0.89
1:A:293:THR:HA	1:D:100:LYS:HD2	1.55	0.89
1:A:25:PRO:HG3	1:D:25:PRO:HD3	1.53	0.88
1:B:24:ASP:HB2	1:B:25:PRO:HD2	1.57	0.86
1:C:222:GLN:HE21	1:C:249:GLN:HB3	1.42	0.84



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:G:24:ASP:HB2	1:G:25:PRO:HD2	1.60	0.84
1:E:42:ARG:HH21	1:E:45:GLU:CD	1.82	0.82
1:G:381:ASP:HB3	1:G:387:ARG:HG3	1.61	0.82
1:H:59:ILE:HD13	1:H:68:ARG:HG3	1.60	0.82
1:C:76:ARG:HH11	1:C:76:ARG:HB2	1.45	0.81
1:D:24:ASP:HB2	1:D:25:PRO:HD2	1.62	0.80
1:A:59:ILE:HD13	1:A:68:ARG:HG3	1.63	0.78
1:H:134:TYR:HB2	1:H:176:ILE:HD11	1.64	0.78
1:E:72:VAL:HG23	4:E:2339:HOH:O	1.84	0.77
1:C:109:ARG:H	1:D:337:GLN:NE2	1.83	0.76
1:E:132:LYS:HA	1:E:176:ILE:HG22	1.68	0.75
1:G:96:HIS:HD2	1:G:98:VAL:H	1.32	0.75
1:H:228:PHE:HB3	1:H:229:PRO:HD3	1.70	0.73
1:A:35:ASP:OD2	1:A:37:VAL:HB	1.89	0.73
1:D:381:ASP:HB3	1:D:387:ARG:HG3	1.70	0.72
1:H:181:GLU:HG3	1:H:215:ASN:O	1.90	0.72
1:C:109:ARG:H	1:D:337:GLN:HE21	1.38	0.71
1:D:196:ILE:HD11	1:D:216:PRO:HB3	1.73	0.71
1:A:365:ALA:HA	1:A:368:ARG:HD3	1.70	0.71
1:B:25:PRO:HD3	1:C:25:PRO:HG3	1.71	0.71
1:A:96:HIS:HD2	1:A:98:VAL:H	1.39	0.70
1:C:96:HIS:HD2	1:C:98:VAL:H	1.37	0.70
1:H:222:GLN:HE21	1:H:249:GLN:HB3	1.56	0.69
1:C:228:PHE:HB3	1:C:229:PRO:HD3	1.75	0.68
1:F:25:PRO:HD3	1:G:25:PRO:HB3	1.75	0.68
1:G:59:ILE:HG12	1:G:68:ARG:HG3	1.76	0.68
1:B:158:MET:HG2	1:B:202:PHE:CZ	2.29	0.68
1:A:377:GLN:NE2	1:C:259:ARG:HE	1.92	0.67
1:F:100:LYS:HD2	1:G:293:THR:HA	1.77	0.66
1:C:222:GLN:NE2	1:C:249:GLN:HB3	2.10	0.66
1:G:109:ARG:H	1:H:337:GLN:NE2	1.94	0.66
1:F:265:LEU:HD23	1:H:265:LEU:HD23	1.78	0.65
1:A:181:GLU:HG3	1:A:215:ASN:O	1.97	0.65
1:F:381:ASP:HB3	1:F:387:ARG:HG3	1.79	0.65
1:E:337:GLN:NE2	1:F:109:ARG:H	1.97	0.63
1:B:259:ARG:HE	1:D:377:GLN:HE21	1.47	0.63
1:E:327:GLN:HG2	4:E:2275:HOH:O	1.99	0.63
1:D:281:GLU:HG2	4:D:2283:HOH:O	1.98	0.63
1:G:76:ARG:HG2	1:G:80:ASP:OD2	2.00	0.62
1:E:24:ASP:HB2	1:E:25:PRO:CD	2.29	0.62
1:D:290:PRO:HG2	1:D:299:VAL:HG13	1.82	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:259:ARG:HE	1:C:377:GLN:NE2	1.98	0.61
1:B:228:PHE:HB3	1:B:229:PRO:HD3	1.83	0.61
1:B:181:GLU:OE2	1:B:220:HIS:HE1	1.83	0.61
1:G:54:HIS:HB2	1:G:57:ASP:OD2	2.00	0.61
1:E:381:ASP:HB3	1:E:387:ARG:HG3	1.83	0.61
1:E:64:SER:OG	1:E:67:GLU:HG3	2.01	0.61
1:A:228:PHE:HB3	1:A:229:PRO:HD3	1.83	0.60
1:C:308:ARG:O	1:C:312:ILE:HG13	2.01	0.60
1:D:158:MET:HG2	1:D:202:PHE:CZ	2.37	0.60
1:H:222:GLN:NE2	1:H:249:GLN:HB3	2.16	0.60
1:G:196:ILE:HG13	1:G:221:GLU:OE2	2.01	0.60
1:A:337:GLN:NE2	1:B:109:ARG:H	2.00	0.60
1:F:228:PHE:HB3	1:F:229:PRO:HD3	1.83	0.60
1:D:96:HIS:HD2	1:D:98:VAL:H	1.48	0.60
1:E:100:LYS:NZ	1:F:366:ALA:O	2.34	0.59
1:F:149:LYS:HE3	4:F:2182:HOH:O	2.02	0.59
1:F:208:ARG:HB3	1:F:210:GLU:OE2	2.02	0.59
1:F:227:ASN:OD1	1:F:229:PRO:HD2	2.03	0.59
1:D:308:ARG:O	1:D:312:ILE:HG13	2.02	0.59
1:D:58:LEU:HD11	1:D:75:PHE:HB2	1.84	0.59
1:B:377:GLN:NE2	1:D:259:ARG:HE	2.01	0.59
1:E:337:GLN:HE21	1:F:109:ARG:H	1.50	0.59
1:C:219:ALA:O	1:C:223:MET:HG3	2.03	0.59
1:G:64:SER:OG	1:G:67:GLU:HG3	2.02	0.59
1:B:31:ARG:HD2	1:B:294:GLU:O	2.03	0.58
1:E:182:PRO:HG2	1:E:196:ILE:HD13	1.86	0.58
1:E:96:HIS:HD2	1:E:98:VAL:H	1.50	0.58
1:H:24:ASP:HB2	1:H:25:PRO:CD	2.34	0.58
1:G:76:ARG:HA	1:G:79:LEU:HD12	1.86	0.57
1:D:182:PRO:HG3	1:D:199:ALA:HB2	1.85	0.57
1:D:59:ILE:HG12	1:D:68:ARG:HG3	1.87	0.57
1:F:116:LEU:HD21	1:F:161:ALA:HB1	1.85	0.57
1:A:109:ARG:H	1:B:337:GLN:HE21	1.52	0.57
1:F:384:LEU:HD21	1:H:265:LEU:HD21	1.86	0.57
1:B:143:ALA:HA	1:B:188:ARG:NH2	2.20	0.57
1:F:40:VAL:HG13	1:F:84:MET:HG3	1.87	0.57
1:H:60:PRO:HA	4:H:2223:HOH:O	2.04	0.56
1:D:2:ASN:ND2	1:D:3:TYR:H	2.03	0.56
1:E:196:ILE:HD11	1:E:216:PRO:HB3	1.86	0.56
1:F:59:ILE:N	1:F:59:ILE:HD12	2.20	0.56
1:A:109:ARG:H	1:B:337:GLN:NE2	2.02	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:F:23:ARG:HH11	1:F:23:ARG:HB3	1.71	0.56
1:G:387:ARG:HG2	4:G:2317:HOH:O	2.05	0.56
1:A:377:GLN:HE21	1:C:259:ARG:HE	1.54	0.56
1:G:109:ARG:H	1:H:337:GLN:HE21	1.53	0.56
1:B:316:ARG:HD3	4:B:2303:HOH:O	2.05	0.56
1:G:387:ARG:HG2	1:G:387:ARG:HH21	1.71	0.55
1:A:218:VAL:HB	1:A:247:ASN:OD1	2.06	0.55
1:C:35:ASP:HB2	4:C:2374:HOH:O	2.05	0.55
1:C:196:ILE:O	1:C:200:LEU:HG	2.06	0.55
1:G:270:TRP:CE2	1:H:146:GLY:HA3	2.41	0.55
1:B:181:GLU:HG3	1:B:215:ASN:O	2.07	0.55
1:F:377:GLN:HE21	1:H:259:ARG:HE	1.54	0.55
1:C:24:ASP:HB2	1:C:25:PRO:CD	2.36	0.55
1:D:222:GLN:HE21	1:D:249:GLN:HB3	1.71	0.55
1:F:58:LEU:C	1:F:59:ILE:HD12	2.26	0.55
1:C:151:VAL:HB	1:D:233:ALA:HB1	1.89	0.55
1:E:25:PRO:HD3	1:H:25:PRO:HG3	1.89	0.55
1:B:38:GLU:OE2	1:B:42:ARG:HD2	2.06	0.55
1:G:36:PRO:O	1:G:40:VAL:HG23	2.07	0.54
1:E:109:ARG:H	1:F:337:GLN:NE2	2.05	0.54
4:F:2340:HOH:O	1:H:266:ARG:HG3	2.08	0.54
1:B:21:GLN:HB3	1:B:29:ALA:HB1	1.88	0.54
1:B:279:GLY:HA2	4:B:2291:HOH:O	2.06	0.54
1:G:219:ALA:O	1:G:223:MET:HG3	2.06	0.54
1:C:14:GLY:HA2	1:C:52:THR:OG1	2.08	0.54
1:E:228:PHE:HB3	1:E:229:PRO:HD3	1.89	0.54
1:B:281:GLU:HG2	4:B:2290:HOH:O	2.08	0.54
1:G:365:ALA:CA	1:G:368:ARG:HD2	2.33	0.54
1:B:37:VAL:HG13	1:B:78:ALA:HB2	1.89	0.54
1:G:228:PHE:HB3	1:G:229:PRO:HD3	1.90	0.54
1:C:151:VAL:HB	1:D:233:ALA:CB	2.39	0.53
1:F:108:ASP:HB3	1:F:110:ASP:OD1	2.07	0.53
1:C:146:GLY:HA3	1:D:270:TRP:CE2	2.43	0.53
1:H:374:ARG:HD2	4:H:2325:HOH:O	2.09	0.53
1:B:259:ARG:HE	1:D:377:GLN:NE2	2.04	0.53
1:E:269:PHE:CD1	1:E:383:LEU:HD13	2.43	0.53
1:A:100:LYS:HD2	1:D:293:THR:HA	1.91	0.53
1:F:218:VAL:HG22	1:F:228:PHE:CE2	2.44	0.53
1:F:158:MET:HG3	1:F:202:PHE:CZ	2.44	0.53
1:E:146:GLY:HA3	1:F:270:TRP:CE2	2.44	0.53
1:A:55:ASP:HB3	1:A:122:ASN:CG	2.28	0.53



	1.5	Interatomic Clash		
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:E:2:ASN:CG	1:E:3:TYR:H	2.12	0.53	
1:E:257:ASP:HB3	1:E:288:PHE:HA	1.89	0.53	
1:B:58:LEU:HD11	1:B:75:PHE:HB2	1.91	0.52	
1:C:96:HIS:CD2	1:C:98:VAL:H	2.22	0.52	
1:G:42:ARG:NH2	1:G:45:GLU:OE2	2.41	0.52	
1:B:312:ILE:O	1:B:316:ARG:HG2	2.10	0.52	
1:B:377:GLN:HE21	1:D:259:ARG:HE	1.56	0.52	
1:E:4:GLN:NE2	1:E:5:PRO:O	2.43	0.52	
1:F:35:ASP:OD2	1:F:37:VAL:HB	2.08	0.52	
1:B:96:HIS:HD2	1:B:98:VAL:HB	1.75	0.52	
1:C:76:ARG:HH11	1:C:76:ARG:CB	2.18	0.52	
1:F:293:THR:HA	1:G:100:LYS:HD2	1.92	0.52	
1:D:257:ASP:HB3	1:D:288:PHE:HA	1.91	0.52	
1:E:196:ILE:CD1	1:E:216:PRO:HB3	2.40	0.51	
1:C:59:ILE:HD13	1:C:68:ARG:HG3	1.91	0.51	
1:A:374:ARG:HD3	4:A:2276:HOH:O	2.10	0.51	
1:E:222:GLN:HE21	1:E:249:GLN:HB3	1.76	0.51	
1:B:222:GLN:NE2	1:B:249:GLN:HB3	2.26	0.51	
1:G:120:ILE:HG23	1:G:168:TYR:CE2	2.46	0.51	
1:A:356:ALA:HA	4:B:2104:HOH:O	2.10	0.51	
1:B:181:GLU:OE2	1:B:220:HIS:CE1	2.62	0.51	
1:A:24:ASP:HB2	1:A:25:PRO:CD	2.41	0.51	
1:G:8:GLU:HB2	4:G:2139:HOH:O	2.10	0.51	
1:G:42:ARG:HA	1:G:42:ARG:NE	2.25	0.51	
1:A:96:HIS:CD2	1:A:98:VAL:H	2.24	0.51	
1:A:222:GLN:HE21	1:A:249:GLN:HB3	1.75	0.51	
1:B:183:LYS:O	1:B:194:PRO:HA	2.11	0.51	
1:D:24:ASP:CB	1:D:25:PRO:HD2	2.39	0.51	
1:G:196:ILE:HG13	1:G:221:GLU:CD	2.32	0.51	
1:E:259:ARG:HE	1:G:377:GLN:NE2	2.09	0.50	
1:F:36:PRO:O	1:F:40:VAL:HG23	2.10	0.50	
1:G:35:ASP:HB3	1:G:38:GLU:HB2	1.91	0.50	
1:G:55:ASP:HB3	1:G:122:ASN:CG	2.30	0.50	
1:A:34:LEU:HD22	4:A:2123:HOH:O	2.11	0.50	
1:C:108:ASP:HB3	1:C:110:ASP:OD1	2.11	0.50	
1:F:377:GLN:NE2	1:H:259:ARG:HE	2.09	0.50	
1:B:23:ARG:HD3	4:B:2175:HOH:O	2.11	0.50	
1:B:24:ASP:HB2	1:B:25:PRO:CD	2.36	0.50	
1:E:27:GLY:HA2	1:H:95:THR:HA	1.94	0.50	
1:H:283:PRO:HG2	4:H:2192:HOH:O	2.10	0.50	
1:B:59:ILE:HD13	1:B:68:ARG:HG3	1.93	0.50	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:152:ABG:HD2	4:E:2203:HOH:O	2.12	0.50
1:G:14:GLY:HA2	1:G:52:THR:OG1	2.12	0.50
1:A:68:ABG:O	1:A:72:VAL:HG23	2.11	0.50
1:A:266:ARG:HG3	4:C:2263:HOH:O	2.12	0.50
1:D:36:PRO:O	1:D:40:VAL:HG23	2.12	0.50
1:G:102:GLY:O	1:G:106:ALA:HB2	2.11	0.50
1:C:183:LYS:O	1:C:194:PRO:HA	2.11	0.50
1:A:377:GLN:NE2	1:C:259:ARG:HH21	2.10	0.49
1:E:196:ILE:HD12	1:E:216:PRO:HG3	1.93	0.49
1:F:97:PRO:CB	1:G:30:THR:HG22	2.42	0.49
1:D:104:PHE:O	1:D:112:ARG:HD2	2.13	0.49
1:H:41:GLN:O	1:H:45:GLU:HG3	2.12	0.49
1:C:327:GLN:OE1	1:H:327:GLN:NE2	2.45	0.49
1:D:222:GLN:NE2	1:D:249:GLN:HB3	2.28	0.49
1:A:24:ASP:HB2	1:A:25:PRO:HD2	1.94	0.49
1:A:259:ARG:HE	1:C:377:GLN:HE21	1.59	0.49
1:H:35:ASP:OD2	1:H:37:VAL:HB	2.12	0.49
1:A:286:PHE:CE1	1:A:306:CYS:HB3	2.47	0.49
1:B:222:GLN:HE21	1:B:249:GLN:HB3	1.77	0.49
1:E:55:ASP:HB3	1:E:122:ASN:CG	2.33	0.49
1:D:327:GLN:HA	1:D:330:LEU:HD12	1.93	0.49
1:C:177:ARG:HH22	1:C:211:LEU:HD23	1.77	0.49
1:B:2:ASN:CG	1:B:3:TYR:H	2.17	0.48
1:G:24:ASP:HB2	1:G:25:PRO:CD	2.39	0.48
1:G:208:ARG:HB3	1:G:210:GLU:OE2	2.12	0.48
1:H:101:ASP:CG	1:H:101:ASP:O	2.52	0.48
1:A:20:TRP:CE3	1:A:289:LYS:HB3	2.48	0.48
1:D:149:LYS:HE3	4:D:2236:HOH:O	2.12	0.48
1:F:294:GLU:HB3	1:F:298:GLY:HA3	1.94	0.48
1:E:227:ASN:OD1	1:E:229:PRO:HD2	2.14	0.48
1:E:259:ARG:HE	1:G:377:GLN:HE21	1.60	0.48
1:G:58:LEU:HB3	1:G:59:ILE:HD12	1.95	0.48
1:C:4:GLN:HB2	4:C:2369:HOH:O	2.13	0.48
1:C:42:ARG:HA	1:C:42:ARG:NE	2.28	0.48
1:D:158:MET:HE1	1:D:193:LEU:HG	1.94	0.48
1:G:343:ALA:HB3	1:H:164:LEU:HD11	1.95	0.48
1:A:219:ALA:O	1:A:223:MET:HG3	2.14	0.48
1:D:381:ASP:CB	1:D:387:ARG:HG3	2.43	0.48
1:G:97:PRO:HB2	1:H:366:ALA:HB1	1.96	0.48
1:G:20:TRP:CH2	1:G:22:GLY:HA2	2.49	0.48
1:E:96:HIS:CD2	1:E:98:VAL:H	2.28	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:182:PRO:HG2	1:C:196:ILE:HA	1.95	0.47
1:A:189:GLY:HA2	1:D:256:GLN:NE2	2.29	0.47
1:E:20:TRP:CE3	1:E:289:LYS:HB3	2.50	0.47
1:A:222:GLN:NE2	1:A:249:GLN:HB3	2.30	0.47
1:D:361:ASP:OD2	1:D:364:ALA:HB2	2.15	0.47
1:A:54:HIS:HB2	1:A:57:ASP:OD2	2.15	0.47
1:B:10:ARG:NH1	4:B:2155:HOH:O	2.45	0.47
1:C:101:ASP:CG	1:C:101:ASP:O	2.52	0.47
1:C:181:GLU:HG3	1:C:215:ASN:O	2.15	0.47
1:E:76:ARG:HH21	1:E:128:GLU:HG2	1.80	0.47
1:E:237:TRP:CZ3	1:F:205:ARG:HD3	2.50	0.47
1:F:377:GLN:NE2	1:H:259:ARG:HH21	2.13	0.47
1:F:97:PRO:HB3	1:G:30:THR:HG22	1.97	0.47
1:G:69:GLU:O	1:G:72:VAL:HG22	2.15	0.47
1:A:51:VAL:O	1:A:86:VAL:HA	2.15	0.47
1:C:196:ILE:HG13	1:C:221:GLU:CD	2.35	0.47
1:D:101:ASP:O	1:D:101:ASP:CG	2.54	0.47
1:D:227:ASN:OD1	1:D:229:PRO:HG2	2.15	0.46
1:G:282:GLY:O	1:G:284:ARG:NH1	2.49	0.46
1:H:281:GLU:HG2	4:H:2312:HOH:O	2.15	0.46
1:H:382:HIS:NE2	1:H:387:ARG:HD3	2.30	0.46
1:F:165:LEU:HB3	1:F:178:PHE:CZ	2.50	0.46
1:A:177:ARG:NH2	4:A:2159:HOH:O	2.48	0.46
1:F:24:ASP:HB2	1:F:25:PRO:CD	2.36	0.46
1:F:55:ASP:HB3	1:F:122:ASN:CG	2.35	0.46
1:G:96:HIS:CD2	1:G:98:VAL:H	2.22	0.46
1:G:228:PHE:CZ	1:G:232:ILE:HD11	2.49	0.46
1:H:15:LEU:HD12	1:H:53:PHE:HB3	1.97	0.46
1:H:24:ASP:HB2	1:H:25:PRO:HD2	1.97	0.46
1:A:257:ASP:HB3	1:A:288:PHE:HA	1.96	0.46
1:D:96:HIS:CD2	1:D:98:VAL:H	2.32	0.46
1:G:101:ASP:CG	1:G:101:ASP:O	2.54	0.46
1:G:218:VAL:HB	1:G:247:ASN:OD1	2.15	0.46
1:H:309:ASN:O	1:H:313:LEU:HG	2.16	0.46
1:G:122:ASN:HB3	1:G:134:TYR:OH	2.15	0.46
1:A:56:ASP:OD2	1:A:92:ASN:HB3	2.16	0.46
4:B:2276:HOH:O	1:D:266:ARG:HG3	2.16	0.46
1:E:244:ILE:O	1:E:285:HIS:HB3	2.15	0.46
1:B:380:MET:HG2	1:D:309:ASN:HD21	1.81	0.46
1:A:246:LEU:HD11	1:A:284:ARG:HB3	1.98	0.45
1:B:20:TRP:O	1:B:31:ARG:NH2	2.49	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:228:PHE:CZ	1:C:232:ILE:HD11	2.51	0.45
1:E:181:GLU:HA	1:E:182:PRO:HD3	1.81	0.45
1:E:219:ALA:O	1:E:223:MET:HG3	2.15	0.45
1:A:205:ARG:HD3	1:B:237:TRP:CZ3	2.51	0.45
1:C:337:GLN:NE2	1:D:109:ARG:H	2.13	0.45
1:D:58:LEU:HD11	1:D:75:PHE:CB	2.46	0.45
1:H:312:ILE:O	1:H:316:ARG:HG2	2.16	0.45
1:C:270:TRP:CE2	1:D:146:GLY:HA3	2.51	0.45
1:D:196:ILE:CD1	1:D:216:PRO:HB3	2.45	0.45
1:H:70:ALA:O	1:H:74:ARG:HG3	2.17	0.45
1:F:183:LYS:HE2	1:F:185:ASN:O	2.17	0.45
1:C:4:GLN:NE2	1:C:5:PRO:HD2	2.32	0.45
1:D:75:PHE:CE2	1:D:79:LEU:HD11	2.52	0.45
1:E:132:LYS:O	1:E:176:ILE:HA	2.16	0.45
1:E:236:LEU:HD21	1:E:241:LEU:HD23	1.98	0.45
1:H:14:GLY:HA2	1:H:52:THR:OG1	2.17	0.45
1:B:251:GLY:HA3	4:B:2275:HOH:O	2.16	0.45
1:F:109:ARG:NH1	1:F:113:ARG:HD2	2.30	0.45
1:H:181:GLU:OE2	1:H:220:HIS:CE1	2.70	0.45
1:E:196:ILE:HG12	1:E:221:GLU:OE1	2.17	0.45
1:G:20:TRP:CZ3	1:G:22:GLY:HA2	2.52	0.45
1:H:58:LEU:HD11	1:H:75:PHE:HB2	1.98	0.45
1:H:96:HIS:CD2	1:H:98:VAL:HG12	2.52	0.45
1:B:42:ARG:NH2	1:B:45:GLU:OE2	2.49	0.45
1:C:177:ARG:NH2	1:C:211:LEU:HD23	2.32	0.45
1:F:58:LEU:HB3	1:F:59:ILE:HD12	1.99	0.45
1:B:88:MET:HG2	1:B:133:VAL:O	2.17	0.45
1:G:345:ASP:OD1	1:G:345:ASP:N	2.47	0.45
1:A:97:PRO:HB3	1:D:30:THR:HG22	1.99	0.45
1:A:120:ILE:HG23	1:A:168:TYR:CE2	2.51	0.45
1:A:384:LEU:HD21	1:C:265:LEU:HD21	1.99	0.45
1:H:41:GLN:HG2	4:H:2208:HOH:O	2.17	0.45
1:G:222:GLN:HE21	1:G:249:GLN:HB3	1.81	0.44
1:B:196:ILE:HG13	1:B:221:GLU:CD	2.37	0.44
1:C:316:ARG:HA	1:C:316:ARG:HD3	1.81	0.44
1:E:259:ARG:HH21	1:G:377:GLN:NE2	2.15	0.44
1:G:336:ASP:N	1:G:336:ASP:OD1	2.50	0.44
1:B:257:ASP:HB3	1:B:288:PHE:HA	1.98	0.44
1:E:15:LEU:HD12	1:E:53:PHE:HB3	2.00	0.44
1:E:24:ASP:HB2	1:E:25:PRO:HD2	1.99	0.44
1:G:35:ASP:O	1:G:38:GLU:HB3	2.16	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:D:70:ALA:O	1:D:74:ARG:HG3	2.17	0.44
1:H:51:VAL:HG13	1:H:84:MET:CE	2.47	0.44
1:B:175:ASP:HB2	4:B:2381:HOH:O	2.17	0.44
1:C:362:VAL:HG23	1:C:363:ASP:N	2.32	0.44
1:D:140:ARG:NH1	1:D:187:PRO:HB2	2.33	0.44
1:C:324:PRO:HG3	1:H:324:PRO:HG3	2.00	0.44
1:E:377:GLN:NE2	1:G:259:ARG:HE	2.16	0.44
1:G:59:ILE:HG21	1:G:68:ARG:HD2	2.00	0.44
1:H:181:GLU:OE2	1:H:220:HIS:HE1	2.00	0.44
1:B:327:GLN:HA	1:B:330:LEU:HD12	2.00	0.44
1:G:35:ASP:HB3	1:G:38:GLU:CB	2.48	0.44
1:A:58:LEU:HD11	1:A:75:PHE:HB2	1.99	0.44
1:A:142:GLY:O	1:A:143:ALA:HB2	2.18	0.44
1:B:140:ARG:NH1	1:B:187:PRO:HB2	2.33	0.44
1:C:309:ASN:O	1:C:313:LEU:HG	2.18	0.44
1:G:251:GLY:HA3	4:G:2116:HOH:O	2.17	0.44
1:G:286:PHE:CE1	1:G:306:CYS:HB3	2.53	0.44
1:B:259:ARG:HH21	1:D:377:GLN:NE2	2.16	0.44
1:B:280:TRP:CH2	1:B:282:GLY:HA3	2.52	0.44
1:D:59:ILE:N	1:D:59:ILE:HD12	2.33	0.44
1:G:286:PHE:CD1	1:G:306:CYS:HB3	2.52	0.44
1:D:2:ASN:N	4:D:2127:HOH:O	2.50	0.43
1:D:96:HIS:CD2	1:D:97:PRO:HD2	2.52	0.43
1:E:109:ARG:H	1:F:337:GLN:HE21	1.67	0.43
1:F:222:GLN:HE21	1:F:249:GLN:HB3	1.82	0.43
1:H:96:HIS:HD2	1:H:98:VAL:H	1.65	0.43
1:H:184:PRO:HD3	4:H:2275:HOH:O	2.17	0.43
1:E:8:GLU:HB2	4:E:2115:HOH:O	2.19	0.43
1:D:42:ARG:HA	1:D:42:ARG:NE	2.34	0.43
1:E:72:VAL:HG23	1:E:73:LYS:N	2.34	0.43
1:G:2:ASN:N	4:G:2131:HOH:O	2.50	0.43
1:D:183:LYS:HG3	1:D:220:HIS:CG	2.54	0.43
1:F:34:LEU:HD11	1:F:38:GLU:HG2	2.01	0.43
1:B:183:LYS:HG2	1:B:184:PRO:HD2	2.01	0.43
1:E:281:GLU:HG2	4:E:2368:HOH:O	2.18	0.43
1:F:320:PHE:O	1:F:326:VAL:HG11	2.19	0.43
1:G:42:ARG:HG3	1:G:300:TRP:CZ2	2.54	0.43
1:C:337:GLN:HE21	1:D:109:ARG:H	1.66	0.43
1:F:219:ALA:O	1:F:223:MET:HG3	2.18	0.43
1:F:215:ASN:HA	1:F:243:HIS:O	2.19	0.42
1:H:34:LEU:HD12	1:H:39:ALA:HB2	1.99	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:246:LEU:HB2	1:D:286:PHE:CD1	2.54	0.42
1:C:12:THR:HG21	1:C:87:PRO:HG2	2.01	0.42
1:E:214:VAL:C	1:E:216:PRO:HD3	2.40	0.42
1:H:65:ASP:O	1:H:69:GLU:HG2	2.19	0.42
1:A:73:LYS:O	1:A:77:GLN:HG2	2.18	0.42
1:C:214:VAL:HG23	1:C:216:PRO:HD3	2.00	0.42
1:D:323:ASP:HB3	1:D:326:VAL:CG2	2.49	0.42
1:F:222:GLN:NE2	1:F:249:GLN:HB3	2.34	0.42
1:G:337:GLN:NE2	1:H:109:ARG:H	2.17	0.42
1:H:132:LYS:HD3	1:H:175:ASP:OD2	2.19	0.42
1:B:265:LEU:HD23	1:D:265:LEU:HD23	2.00	0.42
1:C:203:ILE:HG23	1:C:212:TYR:HB2	2.02	0.42
1:D:17:THR:OG1	1:D:18:VAL:N	2.52	0.42
1:D:387:ARG:NH2	4:D:2403:HOH:O	2.53	0.42
1:F:17:THR:OG1	1:F:18:VAL:N	2.52	0.42
1:F:58:LEU:CB	1:F:59:ILE:HD12	2.49	0.42
1:D:21:GLN:HE21	1:D:21:GLN:HB3	1.67	0.42
1:E:42:ARG:HA	1:E:42:ARG:NE	2.33	0.42
1:G:42:ARG:HH21	1:G:45:GLU:CD	2.22	0.42
1:H:296:ILE:HG23	1:H:297:ASP:N	2.35	0.42
1:C:230:HIS:HB3	4:C:2398:HOH:O	2.19	0.42
1:D:123:ILE:O	1:D:127:VAL:HG23	2.20	0.42
1:D:333:ALA:HB3	1:D:335:LEU:HD23	2.01	0.42
1:E:14:GLY:HA2	1:E:52:THR:OG1	2.19	0.42
1:G:66:THR:HG22	4:G:2325:HOH:O	2.19	0.42
1:A:100:LYS:HD2	1:D:292:ARG:O	2.20	0.42
1:D:206:LEU:O	1:D:209:PRO:HD3	2.20	0.42
1:A:119:THR:O	1:A:123:ILE:HG13	2.20	0.42
1:A:208:ARG:HB3	1:A:210:GLU:OE2	2.20	0.42
1:B:293:THR:HA	1:C:100:LYS:HD2	2.00	0.42
1:B:335:LEU:HD13	1:B:335:LEU:HA	1.91	0.42
1:C:296:ILE:HG23	1:C:297:ASP:N	2.35	0.42
1:D:157:ARG:NE	1:D:157:ARG:HA	2.34	0.42
1:G:312:ILE:O	1:G:316:ARG:HG2	2.20	0.42
1:A:110:ASP:OD1	1:A:111:VAL:N	2.53	0.41
1:C:219:ALA:HA	1:C:249:GLN:HB2	2.01	0.41
1:F:42:ARG:HG3	1:F:300:TRP:CZ2	2.55	0.41
1:H:331:ARG:HD3	4:H:2110:HOH:O	2.20	0.41
1:C:107:ASN:ND2	1:D:372:PHE:HZ	2.18	0.41
1:F:354:ARG:HA	1:F:358:GLU:OE1	2.20	0.41
1:B:219:ALA:O	1:B:223:MET:HG3	2.20	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:28:ASP:HB3	4:C:2350:HOH:O	2.19	0.41
1:D:20:TRP:CE3	1:D:289:LYS:HB3	2.54	0.41
1:D:119:THR:O	1:D:123:ILE:HG13	2.20	0.41
1:F:120:ILE:HG23	1:F:168:TYR:CE2	2.55	0.41
1:G:181:GLU:HA	1:G:182:PRO:HD3	1.88	0.41
1:H:76:ARG:HA	1:H:79:LEU:HD12	2.02	0.41
1:H:334:ARG:HA	1:H:336:ASP:OD1	2.20	0.41
1:A:26:PHE:HA	4:A:2118:HOH:O	2.20	0.41
1:A:42:ARG:HG3	1:A:300:TRP:CZ2	2.56	0.41
1:D:75:PHE:O	1:D:79:LEU:HG	2.21	0.41
1:D:337:GLN:HE21	1:D:337:GLN:HB3	1.68	0.41
1:H:55:ASP:HB3	1:H:122:ASN:CG	2.40	0.41
1:E:212:TYR:CD1	1:E:212:TYR:N	2.89	0.41
1:G:192:LEU:O	1:G:193:LEU:HB2	2.20	0.41
1:A:77:GLN:HG3	4:A:2128:HOH:O	2.21	0.41
1:E:102:GLY:O	1:E:106:ALA:HB2	2.21	0.41
1:A:58:LEU:HD11	1:A:75:PHE:CG	2.56	0.41
1:B:120:ILE:HG23	1:B:168:TYR:CE2	2.56	0.41
1:D:34:LEU:CD2	1:D:38:GLU:HB3	2.51	0.41
1:D:326:VAL:O	1:D:330:LEU:HG	2.21	0.41
1:E:228:PHE:O	1:E:232:ILE:HG12	2.21	0.41
1:F:217:GLU:HG3	1:F:245:ASP:CB	2.51	0.41
1:B:196:ILE:HD11	1:B:216:PRO:HB3	2.03	0.41
1:C:184:PRO:HD3	4:C:2221:HOH:O	2.20	0.41
1:A:184:PRO:HD3	4:A:2185:HOH:O	2.20	0.40
1:B:12:THR:HG21	1:B:87:PRO:HG2	2.03	0.40
1:C:24:ASP:HB2	1:C:25:PRO:HD2	2.03	0.40
1:E:25:PRO:HG3	1:H:25:PRO:HD3	2.03	0.40
1:E:79:LEU:HD23	1:E:84:MET:HB2	2.03	0.40
1:F:21:GLN:HB3	1:F:29:ALA:HB1	2.04	0.40
1:G:8:GLU:O	1:G:8:GLU:HG2	2.22	0.40
1:G:51:VAL:O	1:G:86:VAL:HA	2.20	0.40
1:H:15:LEU:HD12	1:H:53:PHE:CB	2.51	0.40
1:A:337:GLN:HE21	1:B:109:ARG:H	1.67	0.40
1:A:386:ALA:O	1:A:387:ARG:HB2	2.22	0.40
1:E:108:ASP:HB3	1:E:110:ASP:OD1	2.21	0.40
1:E:222:GLN:NE2	1:E:249:GLN:HB3	2.36	0.40
1:F:193:LEU:N	1:F:194:PRO:CD	2.84	0.40
1:H:185:ASN:O	1:H:186:GLU:HB3	2.21	0.40
1:A:55:ASP:OD1	1:A:56:ASP:N	2.54	0.40
1:A:387:ARG:HD2	1:A:387:ARG:HA	1.90	0.40



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:B:183:LYS:HE3	1:B:220:HIS:CD2	2.56	0.40
1:C:40:VAL:HG13	1:C:84:MET:HG3	2.04	0.40
1:C:245:ASP:HB3	1:C:287:ASP:HB3	2.04	0.40
1:D:196:ILE:HG13	1:D:221:GLU:CD	2.42	0.40
1:E:105:THR:OG1	1:E:141:GLU:OE1	2.30	0.40
1:F:40:VAL:CG1	1:F:84:MET:HG3	2.51	0.40
1:H:227:ASN:HB3	1:H:230:HIS:HB2	2.04	0.40
1:D:309:ASN:O	1:D:313:LEU:HG	2.21	0.40
1:G:117:ARG:HD3	1:H:350:LEU:HG	2.03	0.40
1:A:286:PHE:CD1	1:A:306:CYS:HB3	2.56	0.40
1:B:40:VAL:HG13	1:B:84:MET:HG3	2.04	0.40
1:B:101:ASP:O	1:B:101:ASP:CG	2.59	0.40
1:B:184:PRO:HD3	4:B:2248:HOH:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	384/388~(99%)	366~(95%)	17 (4%)	1 (0%)	41	37
1	В	384/388~(99%)	366~(95%)	17 (4%)	1 (0%)	41	37
1	С	384/388~(99%)	367~(96%)	15 (4%)	2(0%)	29	22
1	D	384/388~(99%)	370~(96%)	13 (3%)	1 (0%)	41	37
1	Е	384/388~(99%)	369~(96%)	13 (3%)	2~(0%)	29	22
1	F	384/388~(99%)	367~(96%)	16 (4%)	1 (0%)	41	37
1	G	384/388~(99%)	366~(95%)	17 (4%)	1 (0%)	41	37
1	Н	384/388~(99%)	371 (97%)	11 (3%)	2(0%)	29	22
All	All	3072/3104 (99%)	2942 (96%)	119 (4%)	11 (0%)	34	29



Mol	Chain	Res	Type
1	С	186	GLU
1	С	357	TYR
1	D	186	GLU
1	Е	186	GLU
1	Н	357	TYR
1	А	186	GLU
1	В	186	GLU
1	Е	357	TYR
1	F	186	GLU
1	G	186	GLU
1	Н	186	GLU

All (11) Ramachandran outliers are listed below:

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	296/297~(100%)	294~(99%)	2(1%)	84 89
1	В	296/297~(100%)	292~(99%)	4 (1%)	67 72
1	\mathbf{C}	296/297~(100%)	292~(99%)	4 (1%)	67 72
1	D	296/297~(100%)	294~(99%)	2(1%)	84 89
1	Ε	296/297~(100%)	292~(99%)	4 (1%)	67 72
1	F	296/297~(100%)	291~(98%)	5(2%)	60 65
1	G	296/297~(100%)	293~(99%)	3 (1%)	76 81
1	Н	296/297~(100%)	294 (99%)	2(1%)	84 89
All	All	2368/2376~(100%)	2342 (99%)	26 (1%)	73 78

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	2	ASN
1	А	121	ARG
1	В	65	ASP



Mol	Chain	Res	Type
1	В	73	LYS
1	В	77	GLN
1	В	212	TYR
1	С	76	ARG
1	С	91	THR
1	С	177	ARG
1	С	284	ARG
1	D	34	LEU
1	D	91	THR
1	Е	23	ARG
1	Е	76	ARG
1	Е	91	THR
1	Е	359	ASP
1	F	23	ARG
1	F	77	GLN
1	F	91	THR
1	F	347	LEU
1	F	362	VAL
1	G	23	ARG
1	G	65	ASP
1	G	210	GLU
1	Н	77	GLN
1	Н	345	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	21	GLN
1	А	41	GLN
1	А	96	HIS
1	А	222	GLN
1	А	309	ASN
1	А	327	GLN
1	А	337	GLN
1	А	377	GLN
1	В	41	GLN
1	В	77	GLN
1	В	96	HIS
1	В	220	HIS
1	В	222	GLN
1	В	309	ASN
1	В	337	GLN



Mol	Chain	Res	Type
1	В	377	GLN
1	С	4	GLN
1	С	41	GLN
1	С	96	HIS
1	С	222	GLN
1	С	309	ASN
1	С	327	GLN
1	С	337	GLN
1	С	348	GLN
1	С	377	GLN
1	D	2	ASN
1	D	21	GLN
1	D	41	GLN
1	D	71	HIS
1	D	77	GLN
1	D	96	HIS
1	D	222	GLN
1	D	309	ASN
1	D	327	GLN
1	D	337	GLN
1	D	377	GLN
1	Е	2	ASN
1	Е	41	GLN
1	Ε	96	HIS
1	Ε	222	GLN
1	Ε	309	ASN
1	Е	327	GLN
1	Ε	337	GLN
1	Ε	377	GLN
1	F	41	GLN
1	F	77	GLN
1	F	96	HIS
1	F	222	GLN
1	F	309	ASN
1	F	327	GLN
1	F	337	GLN
1	F	377	GLN
1	G	21	GLN
1	G	41	GLN
1	G	96	HIS
1	G	222	GLN
1	G	309	ASN



Mol	Chain	\mathbf{Res}	Type
1	G	327	GLN
1	G	337	GLN
1	G	348	GLN
1	G	377	GLN
1	Н	41	GLN
1	Н	96	HIS
1	Н	222	GLN
1	Н	309	ASN
1	Н	327	GLN
1	Н	337	GLN
1	Н	377	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)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$Z{>}2$	$OWAB(Å^2)$	Q < 0.9
1	А	386/388~(99%)	-0.53	1 (0%	%) 9	4 95	10, 21, 37, 47	0
1	В	386/388~(99%)	-0.53	0	100	100	10, 20, 37, 49	0
1	С	386/388~(99%)	-0.52	0	100	100	12, 22, 40, 53	0
1	D	386/388~(99%)	-0.56	0	100	100	12, 22, 37, 48	0
1	Ε	386/388~(99%)	-0.57	0	100	100	10, 20, 39, 49	0
1	F	386/388~(99%)	-0.47	0	100	100	12, 24, 44, 55	0
1	G	386/388~(99%)	-0.51	1 (0%	%) 9	4 95	10, 20, 39, 50	0
1	Н	386/388~(99%)	-0.57	0	100	100	8, 20, 35, 47	0
All	All	3088/3104 (99%)	-0.53	2 (0%	%) 9	5 96	8, 21, 38, 55	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	62	GLY	2.7
1	А	386	ALA	2.5

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
2	CO	С	2001	1/1	0.94	0.08	39,39,39,39	0
2	CO	Е	2001	1/1	0.94	0.10	40,40,40,40	0
2	CO	G	2001	1/1	0.94	0.09	40,40,40,40	0
3	MG	F	2002	1/1	0.95	0.17	21,21,21,21	0
2	CO	А	2001	1/1	0.96	0.12	47,47,47,47	0
2	CO	В	2001	1/1	0.96	0.11	$35,\!35,\!35,\!35$	0
3	MG	Н	2002	1/1	0.96	0.22	21,21,21,21	0
2	CO	D	2001	1/1	0.97	0.08	40,40,40,40	0
3	MG	G	2002	1/1	0.97	0.17	13,13,13,13	0
3	MG	D	2002	1/1	0.97	0.17	17,17,17,17	0
2	CO	Н	2001	1/1	0.98	0.10	37,37,37,37	0
3	MG	А	2002	1/1	0.98	0.15	11,11,11,11	0
2	CO	F	2001	1/1	0.98	0.11	40,40,40,40	0
3	MG	С	2002	1/1	0.99	0.12	$15,\!15,\!15,\!15$	0
3	MG	В	2002	1/1	0.99	0.13	18,18,18,18	0
3	MG	Е	2002	1/1	0.99	0.16	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.

