



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2021 – 08:14 PM EST

PDB ID : 3MKV
Title : Crystal structure of amidohydrolase eaj56179
Authors : Patskovsky, Y.; Bonanno, J.; Ozyurt, S.; Sauder, J.M.; Freeman, J.; Wu, B.; Smith, D.; Bain, K.; Rodgers, L.; Wasserman, S.R.; Raushel, F.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-04-15
Resolution : 2.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.16
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) : 2.16

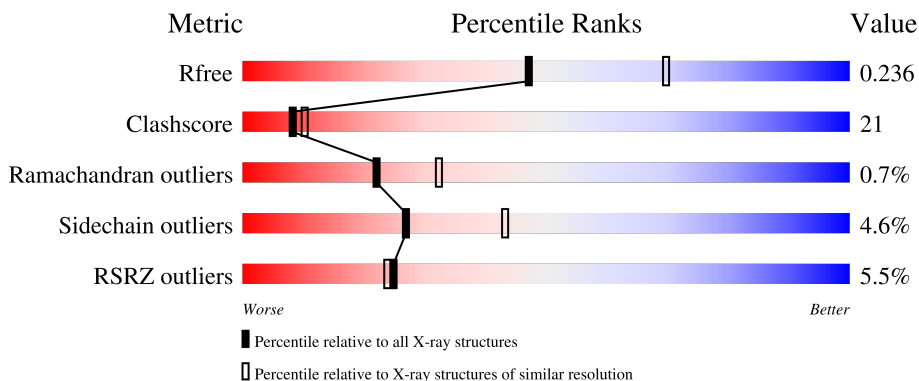
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	A	426	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">68% 26% . .</p>
1	B	426	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 69% 26% . .</p>
1	C	426	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 65% 31% . .</p>
1	D	426	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 68% 26% . .</p>
1	E	426	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 60%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 67% 28% . .</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	426	
1	G	426	
1	H	426	

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	B	427	-	-	X	X
3	SO4	C	427	-	-	X	-
3	SO4	D	428	-	-	X	-
3	SO4	H	429	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25975 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PUTATIVE AMIDOHYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	Total 3147	C 1985	N 561	O 586	S 15	0	6	0
1	B	413	Total 3141	C 1979	N 561	O 586	S 15	0	7	0
1	C	413	Total 3138	C 1974	N 564	O 585	S 15	0	6	0
1	D	413	Total 3121	C 1965	N 557	O 584	S 15	0	3	0
1	E	413	Total 3142	C 1981	N 560	O 586	S 15	0	7	0
1	F	413	Total 3130	C 1973	N 554	O 588	S 15	0	6	0
1	G	413	Total 3131	C 1972	N 559	O 585	S 15	0	5	0
1	H	413	Total 3134	C 1971	N 562	O 586	S 15	0	5	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

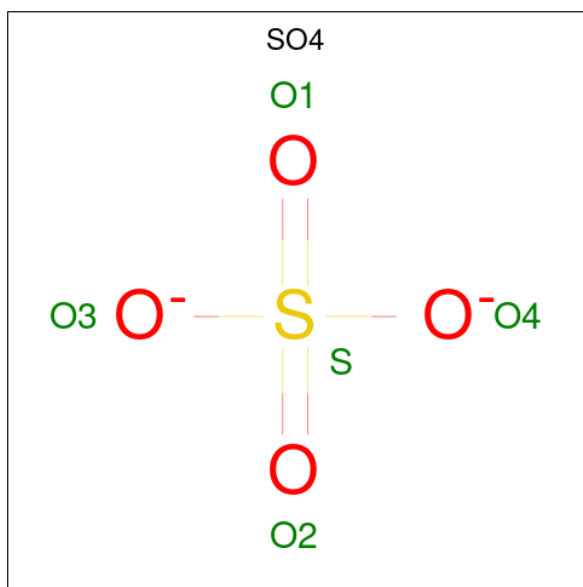
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



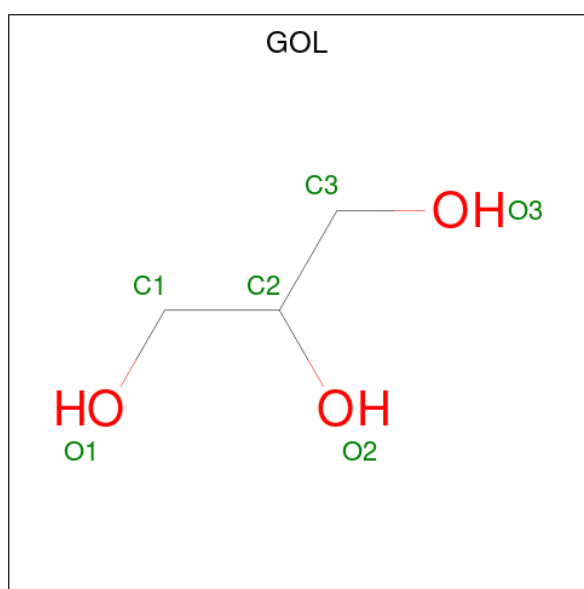
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

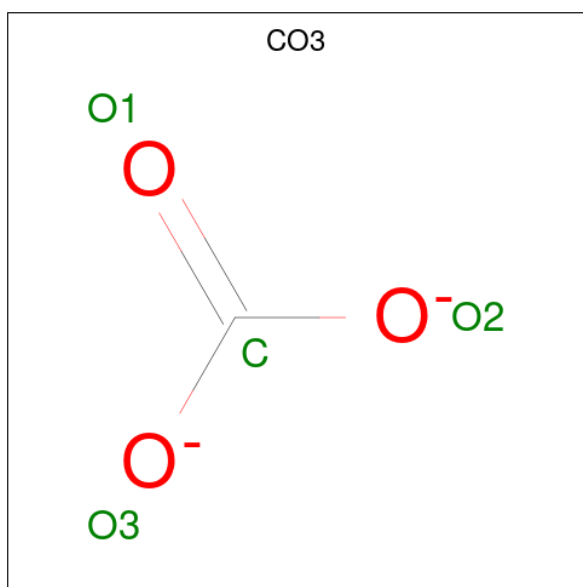
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 4 1 3	0	0
5	G	1	Total C O 4 1 3	0	0

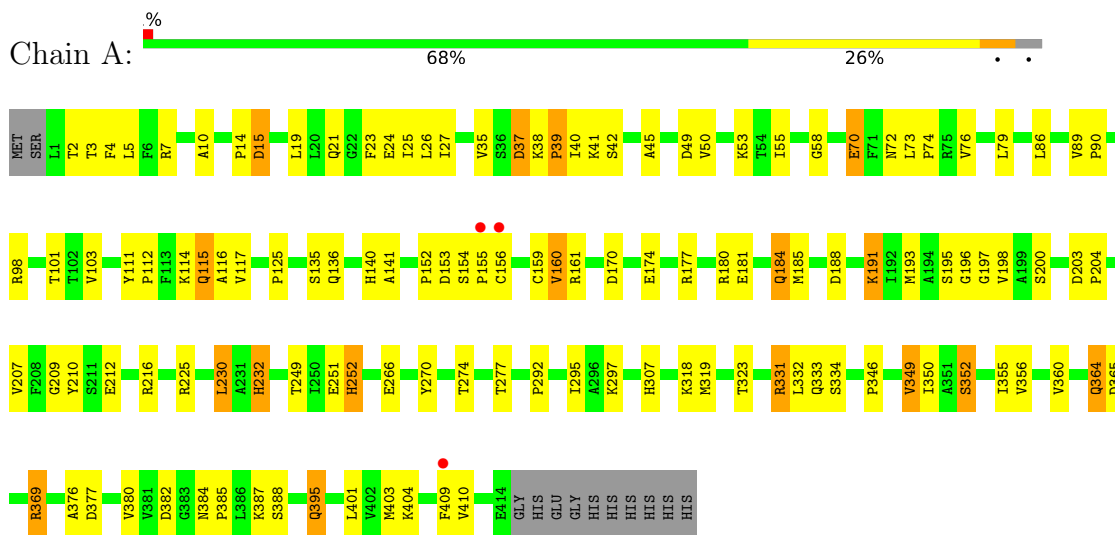
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	135	Total O 135 135	0	0
6	B	124	Total O 124 124	0	0
6	C	111	Total O 111 111	0	0
6	D	99	Total O 99 99	0	0
6	E	90	Total O 90 90	0	0
6	F	88	Total O 88 88	0	0
6	G	75	Total O 75 75	0	0
6	H	68	Total O 68 68	0	0

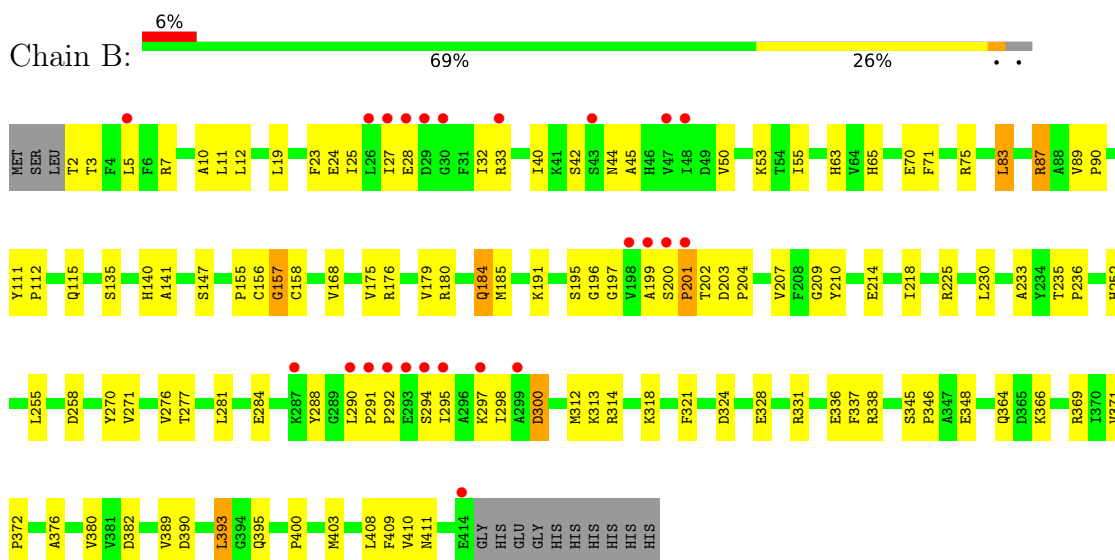
3 Residue-property plots [i](#)

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: PUTATIVE AMIDOHYDROLASE

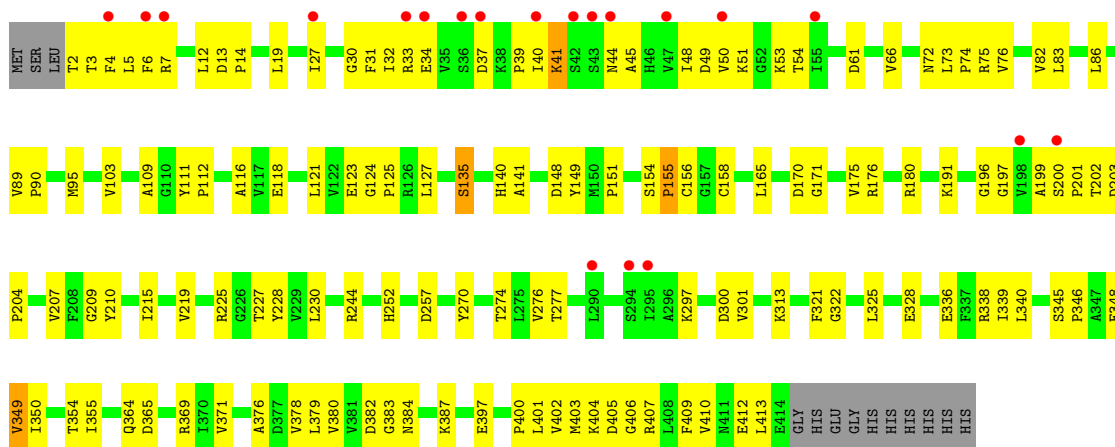


• Molecule 1: PUTATIVE AMIDOHYDROLASE

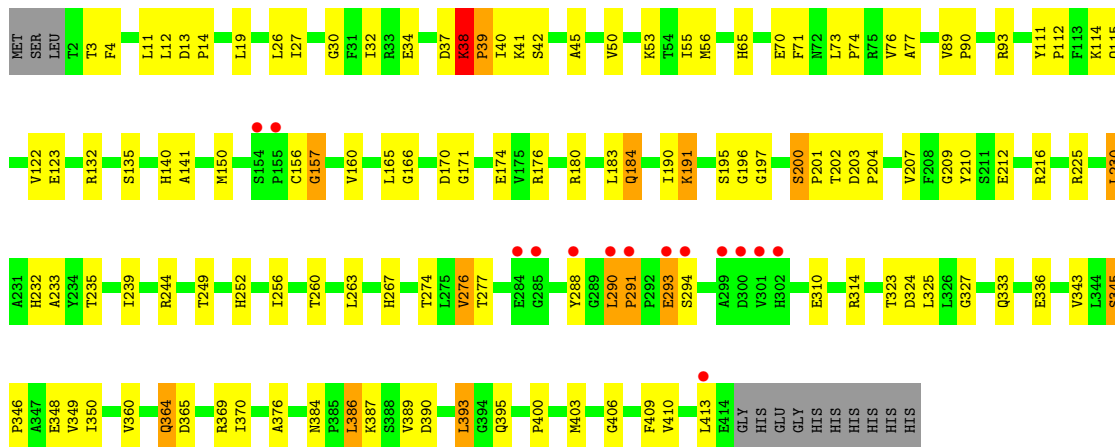


• Molecule 1: PUTATIVE AMIDOHYDROLASE

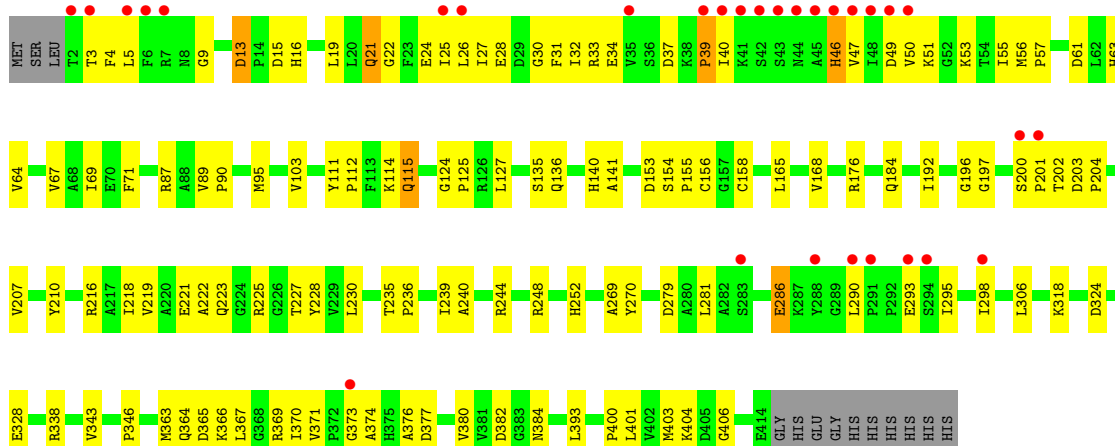




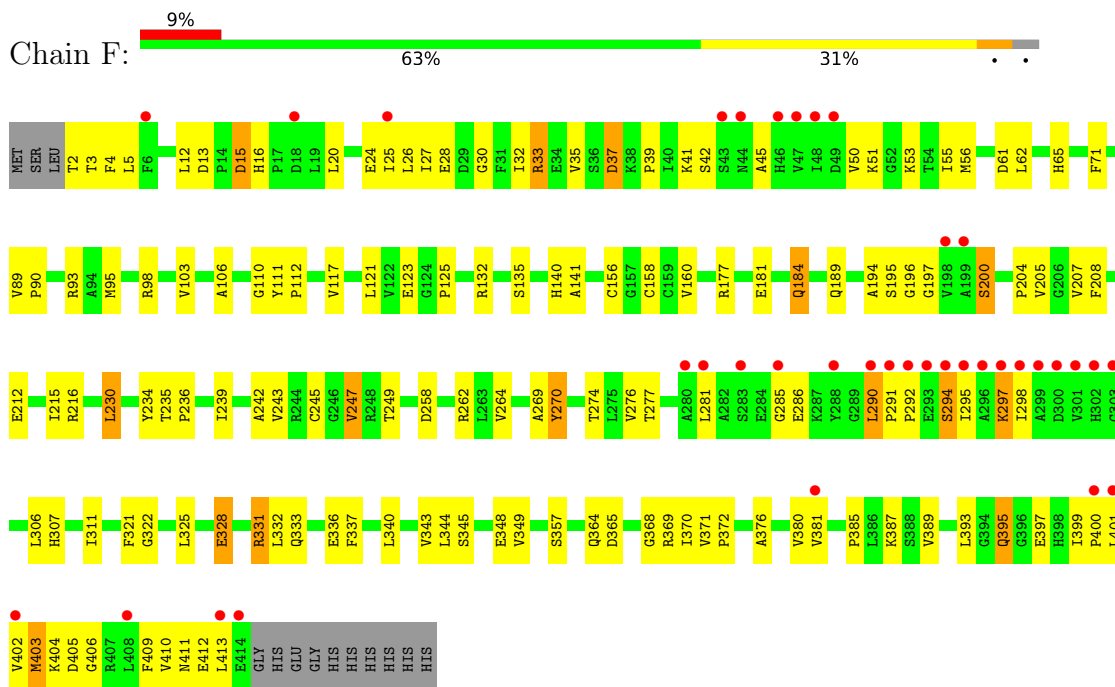
• Molecule 1: PUTATIVE AMIDOHYDROLASE



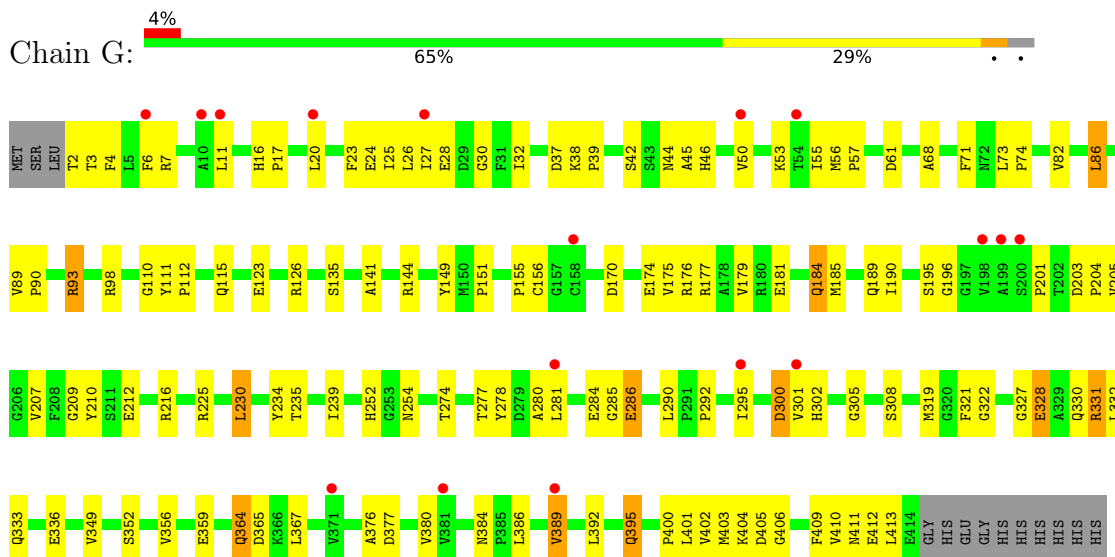
• Molecule 1: PUTATIVE AMIDOHYDROLASE



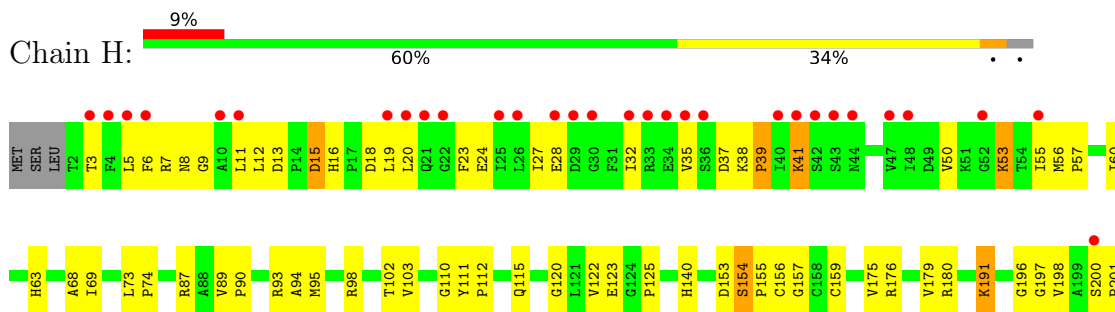
• Molecule 1: PUTATIVE AMIDOHYDROLASE



- Molecule 1: PUTATIVE AMIDOHYDROLASE



- Molecule 1: PUTATIVE AMIDOHYDROLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.02Å 198.60Å 104.29Å 90.00° 107.76° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 49.81 – 2.39	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.00-2.40) 94.7 (49.81-2.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.171 , 0.229 0.179 , 0.236	Depositor DCC
R_{free} test set	3989 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtrriage
Anisotropy	0.319	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25975	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, KCX, CO3, 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/3207	0.52	0/4346
1	B	0.40	0/3204	0.55	0/4342
1	C	0.41	0/3197	0.54	0/4332
1	D	0.38	0/3172	0.53	0/4301
1	E	0.37	0/3205	0.52	0/4343
1	F	0.38	0/3191	0.54	0/4328
1	G	0.37	0/3189	0.53	0/4324
1	H	0.36	0/3191	0.54	0/4327
All	All	0.38	0/25556	0.54	0/34643

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	A	3147	0	3206	109	0
1	B	3141	0	3194	108	0
1	C	3138	0	3193	139	0
1	D	3121	0	3158	131	0
1	E	3142	0	3197	118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3130	0	3168	175	0
1	G	3131	0	3170	137	0
1	H	3134	0	3175	170	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	3	0
3	C	5	0	0	2	0
3	D	10	0	0	2	0
3	E	10	0	0	0	0
3	G	5	0	0	0	0
3	H	15	0	0	4	0
4	C	6	0	8	1	0
4	D	6	0	8	3	0
5	F	4	0	0	0	0
5	G	4	0	0	0	0
6	A	135	0	0	8	0
6	B	124	0	0	6	0
6	C	111	0	0	4	0
6	D	99	0	0	4	0
6	E	90	0	0	9	0
6	F	88	0	0	6	0
6	G	75	0	0	5	0
6	H	68	0	0	6	0
All	All	25975	0	25477	1068	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 21.

All (1068) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:MET:CE	1:H:103:VAL:HG11	1.66	1.25
1:G:7:ARG:HG3	1:G:24:GLU:OE1	1.44	1.12
1:H:53:LYS:HG3	1:H:381:VAL:O	1.47	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:VAL:HG21	1:G:55:ILE:HD11	1.18	1.12
1:G:376:ALA:HB1	1:G:403:MET:CE	1.78	1.11
1:B:3:THR:HG22	1:B:45:ALA:CB	1.78	1.11
1:A:140:HIS:CE1	1:A:197:GLY:HA3	1.85	1.09
1:B:140:HIS:ND1	1:B:197:GLY:HA3	1.67	1.09
1:E:286:GLU:HG2	1:E:295:ILE:HD13	1.35	1.09
1:B:3:THR:HG22	1:B:45:ALA:HB1	1.36	1.07
1:H:95:MET:HE3	1:H:103:VAL:HG11	1.27	1.07
1:F:140:HIS:ND1	1:F:197:GLY:HA3	1.72	1.04
1:G:376:ALA:HB1	1:G:403:MET:HE2	1.39	1.03
1:D:50:VAL:HG21	1:D:55:ILE:HD11	1.39	1.03
1:A:376:ALA:HB1	1:A:403:MET:HE3	1.41	1.03
1:H:292:PRO:HA	1:H:295:ILE:HD12	1.40	1.02
1:F:331:ARG:HH11	1:F:332:LEU:HD21	1.20	1.01
1:B:409[A]:PHE:CD1	1:B:410:VAL:HG23	1.96	1.01
1:D:276:VAL:CG2	1:D:336:GLU:HB2	1.91	1.00
1:F:123:GLU:OE1	1:F:409[B]:PHE:HD1	1.44	1.00
1:C:34:GLU:OE2	1:C:40:ILE:HD12	1.60	1.00
1:B:140:HIS:CE1	1:B:197:GLY:HA3	1.98	0.99
1:B:369:ARG:NH2	1:B:371:VAL:HG11	1.76	0.99
1:F:276:VAL:HG23	1:F:336:GLU:OE2	1.63	0.99
1:H:50:VAL:HG21	1:H:55:ILE:HD11	1.45	0.98
1:D:135:SER:HB2	1:D:141:ALA:HB3	1.44	0.97
1:H:27:ILE:CD1	1:H:32:ILE:HD13	1.94	0.97
1:B:3:THR:CG2	1:B:45:ALA:HB2	1.92	0.97
1:F:286:GLU:HG2	1:F:295:ILE:HD13	1.49	0.95
1:H:389:VAL:O	1:H:389:VAL:HG13	1.65	0.94
1:D:37:ASP:O	1:D:39:PRO:HD3	1.67	0.94
1:E:286:GLU:HG2	1:E:295:ILE:CD1	1.96	0.94
1:F:140:HIS:CE1	1:F:197:GLY:HA3	2.02	0.93
1:F:123:GLU:OE1	1:F:409[B]:PHE:CD1	2.21	0.93
1:F:286:GLU:HG2	1:F:295:ILE:CD1	1.98	0.93
1:F:380:VAL:O	1:F:400:PRO:HD2	1.68	0.92
1:H:292:PRO:HA	1:H:295:ILE:CD1	2.00	0.92
1:B:196:GLY:HA3	1:B:204:PRO:O	1.69	0.92
1:D:19:LEU:HD11	1:D:384:ASN:OD1	1.69	0.91
1:F:328:GLU:H	1:F:328:GLU:CD	1.71	0.91
1:G:2:THR:HG22	1:G:3:THR:H	1.33	0.91
1:C:27:ILE:HG21	1:C:403:MET:HE3	1.53	0.90
1:G:27:ILE:HG21	1:G:403:MET:HE3	1.54	0.89
1:G:7:ARG:CG	1:G:24:GLU:OE1	2.20	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:THR:CG2	1:B:45:ALA:CB	2.50	0.88
1:E:380:VAL:HB	1:E:401:LEU:HB3	1.54	0.88
1:E:135:SER:HB2	1:E:141:ALA:HB3	1.53	0.88
1:E:95:MET:CE	1:E:103:VAL:HG11	2.04	0.88
1:D:409[A]:PHE:CD1	1:D:410:VAL:HG23	2.09	0.87
1:A:376:ALA:HB1	1:A:403:MET:CE	2.04	0.86
1:A:274:THR:O	1:A:277:THR:HG22	1.76	0.86
1:F:331:ARG:NH1	1:F:332:LEU:HD21	1.89	0.86
1:B:201:PRO:HD2	6:B:520:HOH:O	1.76	0.85
1:A:140:HIS:HB3	1:A:193:MET:HG3	1.59	0.85
1:H:321:PHE:CZ	1:H:336:GLU:HB3	2.11	0.85
1:E:95:MET:HE2	1:E:103:VAL:HG11	1.59	0.85
1:F:204:PRO:HD2	1:F:207:VAL:HG21	1.59	0.84
1:F:371:VAL:CG2	1:F:372:PRO:HD2	2.06	0.84
1:G:50:VAL:CG2	1:G:55:ILE:HD11	2.06	0.84
1:E:135:SER:CB	1:E:141:ALA:HB3	2.06	0.84
1:E:346:PRO:HD3	6:E:466:HOH:O	1.77	0.84
1:H:378:VAL:HB	1:H:403:MET:CE	2.07	0.84
1:G:292:PRO:O	1:G:295:ILE:HG22	1.76	0.84
1:F:32:ILE:HD13	1:F:370:ILE:HG23	1.59	0.83
1:H:212:GLU:HB3	1:H:216[B]:ARG:NH2	1.92	0.83
1:D:276:VAL:HG21	1:D:336:GLU:HB2	1.59	0.83
1:E:25:ILE:CD1	1:E:55:ILE:HG21	2.09	0.83
1:F:371:VAL:HG22	1:F:372:PRO:HD2	1.57	0.83
1:G:6:PHE:HB2	1:G:25:ILE:HB	1.60	0.83
1:H:38:LYS:O	1:H:39:PRO:O	1.95	0.83
1:H:378:VAL:HB	1:H:403:MET:HE2	1.58	0.83
1:A:346:PRO:O	1:A:350:ILE:HD13	1.79	0.83
1:G:380:VAL:HB	1:G:401:LEU:HB3	1.61	0.82
1:C:3:THR:CG2	1:C:45:ALA:HB2	2.09	0.82
1:A:50:VAL:HG21	1:A:55:ILE:HD11	1.61	0.82
1:B:3:THR:HG21	1:B:45:ALA:HB2	1.61	0.81
1:C:140:HIS:ND1	1:C:197:GLY:HA3	1.95	0.81
1:B:390:ASP:HA	1:B:393:LEU:HD22	1.62	0.81
1:F:95:MET:CE	1:F:103:VAL:HG11	2.09	0.81
1:G:7:ARG:HG3	1:G:24:GLU:CD	2.00	0.81
1:E:19:LEU:HD12	1:E:384:ASN:ND2	1.96	0.81
1:C:34:GLU:OE2	1:C:40:ILE:CD1	2.29	0.81
1:C:12:LEU:HD23	1:C:12:LEU:C	2.00	0.81
1:D:19:LEU:CD1	1:D:384:ASN:OD1	2.29	0.81
1:H:285:GLY:O	1:H:290:LEU:HB3	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:HG12	1:D:53:LYS:H	1.46	0.80
1:D:32:ILE:HD12	1:D:370:ILE:HG23	1.62	0.80
1:H:95:MET:HE1	1:H:125:PRO:HG2	1.63	0.80
1:D:50:VAL:HG21	1:D:55:ILE:CD1	2.12	0.79
1:A:135:SER:HB2	1:A:141:ALA:HB3	1.63	0.79
1:A:42:SER:HB2	1:A:45:ALA:HB2	1.65	0.79
1:H:343:VAL:CG1	1:H:343:VAL:O	2.30	0.79
1:E:140:HIS:ND1	1:E:197:GLY:HA3	1.99	0.78
1:H:140:HIS:ND1	1:H:197:GLY:HA3	1.98	0.78
1:B:71:PHE:HB3	1:B:290:LEU:HD12	1.64	0.78
1:A:200:SER:HB2	1:A:203:ASP:OD1	1.83	0.78
1:G:380:VAL:O	1:G:400:PRO:HD2	1.82	0.78
1:C:380:VAL:O	1:C:400:PRO:HD2	1.84	0.78
1:G:328:GLU:H	1:G:328:GLU:CD	1.87	0.78
1:F:328:GLU:N	1:F:328:GLU:CD	2.35	0.78
1:E:4:PHE:O	1:E:26:LEU:HD12	1.84	0.78
1:C:400:PRO:HB2	1:C:413:LEU:HD21	1.66	0.78
1:E:50:VAL:HG12	1:E:53:LYS:H	1.48	0.77
1:C:409:PHE:CD1	1:C:410:VAL:HG23	2.20	0.77
1:B:345:SER:OG	1:B:348:GLU:HG3	1.84	0.77
1:H:346:PRO:HB2	1:H:386:LEU:O	1.82	0.77
1:F:196:GLY:HA3	1:F:204:PRO:O	1.84	0.77
1:C:3:THR:HG22	1:C:45:ALA:CB	2.15	0.77
1:A:37:ASP:O	1:A:39:PRO:HD3	1.85	0.76
1:H:140:HIS:CE1	1:H:197:GLY:HA3	2.21	0.76
1:H:343:VAL:HG12	1:H:343:VAL:O	1.84	0.76
1:D:263:LEU:HD12	1:D:267:HIS:HD2	1.50	0.76
1:D:263:LEU:HD12	1:D:267:HIS:CD2	2.21	0.76
1:C:5:LEU:HD23	1:C:5:LEU:C	2.05	0.75
1:E:25:ILE:HD11	1:E:55:ILE:HG21	1.68	0.75
1:F:50:VAL:HG12	1:F:53:LYS:H	1.50	0.75
1:G:176:ARG:HD3	6:G:436:HOH:O	1.85	0.75
1:F:71:PHE:HB3	1:F:290:LEU:HD23	1.67	0.75
1:E:380:VAL:O	1:E:400:PRO:HD2	1.85	0.75
1:H:50:VAL:CG2	1:H:55:ILE:HD11	2.16	0.75
1:F:276:VAL:HG21	1:F:336:GLU:HB2	1.67	0.75
1:E:235:THR:O	1:E:239:ILE:HG13	1.87	0.74
1:E:363:MET:HE2	1:E:363:MET:HA	1.69	0.74
1:F:376:ALA:HB3	1:F:406:GLY:N	2.02	0.74
1:C:412:GLU:O	1:C:413:LEU:HD23	1.87	0.74
1:G:319:MET:O	1:G:356:VAL:HG11	1.86	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PRO:HA	1:A:388:SER:O	1.86	0.74
1:F:395:GLN:OE1	1:F:395:GLN:HA	1.86	0.74
1:A:225:ARG:HA	1:C:207:VAL:HG23	1.68	0.74
1:G:376:ALA:CB	1:G:403:MET:HE2	2.15	0.74
1:G:42:SER:OG	1:G:44:ASN:HB2	1.88	0.74
1:E:64:VAL:HG11	1:E:95:MET:CE	2.18	0.74
1:H:321:PHE:HZ	1:H:336:GLU:HB3	1.50	0.74
1:D:40:ILE:HG13	1:D:41:LYS:N	2.03	0.74
1:A:2:THR:HG23	1:A:2:THR:O	1.86	0.73
1:E:64:VAL:HG11	1:E:95:MET:HE3	1.70	0.73
1:F:380:VAL:HB	1:F:401:LEU:HB3	1.69	0.73
1:C:176:ARG:HD3	6:C:519:HOH:O	1.88	0.73
1:D:204:PRO:O	1:D:207:VAL:HG12	1.87	0.73
1:H:19:LEU:HD13	1:H:384:ASN:ND2	2.03	0.73
1:F:27:ILE:HG21	1:F:403:MET:HE1	1.70	0.73
1:C:95:MET:CE	1:C:103:VAL:HG11	2.19	0.73
1:D:40:ILE:HG13	1:D:41:LYS:H	1.53	0.72
1:B:71:PHE:HB3	1:B:290:LEU:CD1	2.19	0.72
1:F:331:ARG:HH11	1:F:332:LEU:CD2	2.00	0.72
1:A:270:TYR:CE1	1:A:318:LYS:HE2	2.24	0.72
1:H:95:MET:HE2	1:H:103:VAL:HG11	1.70	0.72
1:D:400:PRO:HB2	1:D:413:LEU:CD2	2.20	0.72
1:G:254:ASN:ND2	1:G:301:VAL:HG13	2.04	0.72
1:F:401:LEU:C	1:F:401:LEU:HD23	2.09	0.72
1:E:196:GLY:HA3	1:E:204:PRO:O	1.90	0.71
1:G:25:ILE:CD1	1:G:55:ILE:HG21	2.19	0.71
1:H:27:ILE:CD1	1:H:32:ILE:CD1	2.68	0.71
1:C:346:PRO:O	1:C:350:ILE:HD13	1.91	0.71
1:G:331:ARG:HD3	1:G:332:LEU:CD2	2.19	0.71
1:A:15:ASP:OD2	1:A:15:ASP:N	2.21	0.71
1:C:3:THR:HG22	1:C:45:ALA:HB2	1.71	0.71
1:B:380:VAL:O	1:B:400:PRO:HD2	1.91	0.70
1:F:30:GLY:HA2	1:F:406:GLY:HA3	1.73	0.70
1:G:135:SER:HB2	1:G:141:ALA:HB3	1.73	0.70
1:C:376:ALA:HB1	1:C:403:MET:CE	2.21	0.70
1:G:27:ILE:CG2	1:G:403:MET:HE3	2.21	0.70
1:E:240:ALA:O	1:E:244[A]:ARG:HG3	1.91	0.70
1:F:276:VAL:CG2	1:F:336:GLU:HB2	2.22	0.70
1:H:27:ILE:HD13	1:H:32:ILE:HD13	1.72	0.70
1:F:51:LYS:HA	1:F:51:LYS:HE2	1.73	0.70
1:H:212:GLU:HB3	1:H:216[B]:ARG:HH21	1.54	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLY:O	1:C:404[A]:LYS:HE2	1.92	0.69
1:C:50:VAL:HG12	1:C:53:LYS:HB2	1.75	0.69
1:B:369:ARG:HH21	1:B:371:VAL:HG11	1.54	0.69
1:C:27:ILE:HD12	1:C:32:ILE:HD13	1.74	0.69
1:F:71:PHE:CE1	1:F:328:GLU:OE2	2.45	0.69
1:H:38:LYS:O	1:H:39:PRO:C	2.31	0.69
1:H:95:MET:HE3	1:H:103:VAL:CG1	2.15	0.69
1:A:140:HIS:ND1	1:A:197:GLY:HA3	2.06	0.69
1:D:263:LEU:CD1	1:D:267:HIS:CD2	2.75	0.69
1:D:291:PRO:HB3	1:D:293:GLU:OE2	1.92	0.69
1:H:53:LYS:HD2	1:H:382:ASP:HA	1.74	0.68
1:C:3:THR:HG21	1:C:45:ALA:HB2	1.74	0.68
1:C:196:GLY:HA3	1:C:204:PRO:O	1.94	0.68
1:G:27:ILE:HG13	1:G:403:MET:CE	2.23	0.68
1:D:400:PRO:HB2	1:D:413:LEU:HD23	1.74	0.68
1:D:50:VAL:HG11	1:D:53:LYS:O	1.94	0.68
1:G:50:VAL:HG21	1:G:55:ILE:CD1	2.11	0.68
1:C:165:LEU:HB2	4:C:428:GOL:H2	1.75	0.68
1:C:83:LEU:HD11	1:H:115:GLN:NE2	2.09	0.68
1:B:369:ARG:HG2	1:B:371:VAL:HG13	1.76	0.68
1:D:140:HIS:CE1	1:D:197:GLY:HA3	2.28	0.68
1:H:201:PRO:HA	1:H:293:GLU:OE1	1.93	0.68
1:A:153:ASP:HB2	6:A:476:HOH:O	1.94	0.67
1:A:160:VAL:HG13	1:C:148:ASP:O	1.94	0.67
1:H:37:ASP:OD2	1:H:38:LYS:HD2	1.93	0.67
1:F:95:MET:HE2	1:F:103:VAL:HG11	1.76	0.67
1:H:27:ILE:HD11	1:H:32:ILE:CD1	2.23	0.67
1:C:95:MET:HE1	1:C:103:VAL:HG11	1.76	0.67
1:F:71:PHE:HE1	1:F:328:GLU:HG2	1.59	0.67
1:B:27:ILE:CD1	1:B:32:ILE:HD13	2.25	0.67
1:E:27:ILE:HG21	1:E:403:MET:HE1	1.76	0.67
1:H:15:ASP:N	1:H:15:ASP:OD2	2.27	0.67
1:D:12:LEU:HD23	1:D:12:LEU:C	2.15	0.67
1:C:156:CYS:SG	1:H:156:CYS:O	2.50	0.67
1:H:380:VAL:HB	1:H:401:LEU:HB3	1.77	0.66
1:H:53:LYS:CG	1:H:381:VAL:O	2.36	0.66
1:H:19:LEU:CD1	1:H:386:LEU:HD12	2.25	0.66
1:E:13:ASP:C	1:E:13:ASP:OD1	2.33	0.66
1:G:111:TYR:N	1:G:112:PRO:CD	2.59	0.66
1:D:93:ARG:NH2	1:D:123:GLU:OE2	2.29	0.66
1:H:321:PHE:CE1	1:H:336:GLU:CG	2.79	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:HIS:CE1	1:E:197:GLY:HA3	2.30	0.66
1:A:50:VAL:HG12	1:A:53:LYS:HB2	1.78	0.66
1:B:408:LEU:HD13	1:B:411:ASN:HD22	1.60	0.66
1:E:27:ILE:HG13	1:E:403:MET:HE1	1.76	0.66
1:H:24:GLU:OE1	1:H:39:PRO:HB3	1.95	0.66
1:F:328:GLU:N	1:F:328:GLU:OE1	2.28	0.66
1:H:123:GLU:OE1	1:H:409:PHE:HE2	1.79	0.66
1:C:50:VAL:HG12	1:C:53:LYS:H	1.60	0.65
1:H:270:TYR:CE1	1:H:318:LYS:HE2	2.31	0.65
1:H:321:PHE:CE1	1:H:336:GLU:HG3	2.31	0.65
1:F:25:ILE:HG23	1:F:35:VAL:HG22	1.77	0.65
1:F:33:ARG:HH11	1:F:33:ARG:HA	1.60	0.65
1:F:50:VAL:HG12	1:F:53:LYS:N	2.11	0.65
1:B:236:PRO:HD3	1:B:255:LEU:O	1.96	0.65
1:G:277:THR:O	1:G:281:LEU:HG	1.97	0.65
1:F:135:SER:HB2	1:F:141:ALA:HB3	1.77	0.65
1:H:112:PRO:HA	1:H:115:GLN:HG2	1.78	0.65
1:E:328:GLU:OE1	1:E:328:GLU:N	2.23	0.65
1:H:389:VAL:O	1:H:389:VAL:CG1	2.39	0.65
1:B:27:ILE:HD12	1:B:32:ILE:HD13	1.79	0.65
1:C:49:ASP:OD2	1:C:51:LYS:CG	2.45	0.65
1:D:27:ILE:HD11	1:D:32:ILE:HD13	1.78	0.65
1:H:255:LEU:HD11	1:H:301:VAL:HG12	1.78	0.65
1:H:364:GLN:O	1:H:365:ASP:HB2	1.96	0.65
1:C:412:GLU:C	1:C:413:LEU:HD23	2.17	0.65
1:A:319:MET:O	1:A:356:VAL:HG11	1.96	0.64
1:D:290:LEU:C	1:D:290:LEU:HD13	2.17	0.64
1:E:200:SER:HB2	1:E:201:PRO:HD2	1.80	0.64
1:C:49:ASP:OD2	1:C:51:LYS:HG3	1.97	0.64
1:B:180:ARG:NH1	1:D:170:ASP:OD1	2.28	0.64
1:H:156:CYS:CB	1:H:159:CYS:O	2.45	0.64
1:H:300:ASP:N	1:H:300:ASP:OD2	2.30	0.64
1:F:50:VAL:O	1:F:51:LYS:HB2	1.98	0.64
1:H:196:GLY:HA3	1:H:204:PRO:O	1.97	0.64
1:E:376:ALA:HB1	1:E:403:MET:CE	2.27	0.64
1:G:327:GLY:O	1:G:330:GLN:HG3	1.97	0.64
1:B:284:GLU:O	1:B:284:GLU:HG3	1.97	0.64
1:F:331:ARG:HD3	1:F:332:LEU:CD2	2.27	0.64
1:G:400:PRO:HB2	1:G:413:LEU:CD1	2.28	0.64
1:A:200:SER:CB	1:A:203:ASP:OD1	2.45	0.64
1:D:216[A]:ARG:HD3	6:D:525:HOH:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244[A]:ARG:NE	3:H:429:SO4:O3	2.29	0.64
1:H:198:VAL:N	3:H:427:SO4:O3	2.28	0.64
1:E:50:VAL:HG21	1:E:55:ILE:HD11	1.80	0.64
1:E:15:ASP:OD2	1:E:16:HIS:ND1	2.31	0.64
1:G:285:GLY:O	1:G:290:LEU:HB3	1.97	0.64
1:G:349:VAL:O	1:G:352:SER:HB2	1.98	0.64
1:D:37:ASP:O	1:D:39:PRO:CD	2.44	0.63
1:G:123:GLU:OE2	1:G:409[B]:PHE:CE1	2.51	0.63
1:H:123:GLU:OE1	1:H:409:PHE:CE2	2.51	0.63
1:E:95:MET:HE1	1:E:103:VAL:HG11	1.78	0.63
1:B:209:GLY:O	1:B:210:TYR:HB2	1.98	0.63
1:B:111:TYR:N	1:B:112:PRO:CD	2.62	0.63
1:C:61:ASP:OD1	1:C:322:GLY:HA2	1.98	0.63
1:D:140:HIS:ND1	1:D:197:GLY:HA3	2.12	0.63
1:D:212:GLU:OE2	1:D:216[A]:ARG:NH2	2.32	0.63
1:D:71:PHE:HB3	1:D:290:LEU:HD23	1.81	0.63
1:F:276:VAL:CG2	1:F:336:GLU:CA	2.77	0.63
1:G:50:VAL:O	1:G:53:LYS:HD2	1.98	0.63
1:B:409[A]:PHE:CE1	1:B:410:VAL:HG23	2.33	0.62
1:D:89:VAL:HB	1:D:90:PRO:HD3	1.80	0.62
1:E:136:GLN:HG2	6:E:464:HOH:O	1.98	0.62
1:F:235:THR:O	1:F:239:ILE:HG13	1.99	0.62
1:G:331:ARG:HD3	1:G:332:LEU:HD21	1.82	0.62
1:A:114[B]:LYS:NZ	1:A:188:ASP:OD1	2.32	0.62
1:C:349:VAL:HG22	1:C:350:ILE:HD12	1.81	0.62
6:B:495:HOH:O	1:D:171:GLY:HA2	1.99	0.62
1:F:98:ARG:NH2	1:F:333:GLN:OE1	2.32	0.62
1:G:401:LEU:HD23	1:G:402:VAL:N	2.15	0.62
1:D:276:VAL:HG22	1:D:336:GLU:HB2	1.79	0.62
1:C:397:GLU:N	1:C:397:GLU:OE1	2.26	0.62
1:G:98:ARG:HD3	1:G:395:GLN:OE1	2.00	0.62
1:E:27:ILE:HG13	1:E:403:MET:CE	2.30	0.62
1:C:50:VAL:CG1	1:C:53:LYS:HB2	2.30	0.62
1:D:345:SER:O	1:D:348:GLU:N	2.30	0.62
1:A:401:LEU:HA	1:A:410:VAL:O	1.99	0.62
1:H:11:LEU:HD22	1:H:20:LEU:HD12	1.82	0.62
1:C:369:ARG:HD2	1:C:371:VAL:HG11	1.82	0.61
1:C:73:LEU:HD13	1:C:165:LEU:HD12	1.82	0.61
1:G:285:GLY:O	1:G:290:LEU:CB	2.48	0.61
1:H:255:LEU:CD1	1:H:301:VAL:HG12	2.31	0.61
1:A:323:THR:HG21	1:A:333:GLN:HG3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ASN:ND2	1:C:75:ARG:HB2	2.14	0.61
1:F:93:ARG:NH2	1:F:123:GLU:OE2	2.33	0.61
1:H:19:LEU:HD22	1:H:384:ASN:HD22	1.64	0.61
1:D:364:GLN:O	1:D:365:ASP:HB2	2.00	0.61
1:D:50:VAL:HG12	1:D:53:LYS:N	2.16	0.61
1:H:285:GLY:O	1:H:290:LEU:CB	2.47	0.61
1:C:376:ALA:HB1	1:C:403:MET:HE2	1.81	0.61
1:F:274:THR:O	1:F:277:THR:HG22	2.01	0.61
1:H:111:TYR:N	1:H:112:PRO:CD	2.63	0.61
1:A:364:GLN:O	1:A:365:ASP:HB2	2.00	0.61
1:D:195:SER:HB3	1:D:233:ALA:HA	1.82	0.61
1:B:175:VAL:O	1:B:179:VAL:HG23	2.01	0.61
1:F:95:MET:HE1	1:F:125:PRO:HG2	1.82	0.61
1:F:286:GLU:CG	1:F:295:ILE:HD13	2.28	0.61
1:G:37:ASP:OD2	1:G:38:LYS:N	2.33	0.61
1:D:170:ASP:HB2	6:D:504:HOH:O	2.00	0.61
1:A:27:ILE:N	1:A:27:ILE:HD12	2.15	0.61
1:D:140:HIS:HD1	1:D:200:SER:HG	1.46	0.61
1:H:376:ALA:HB3	1:H:406:GLY:N	2.16	0.60
1:E:53:LYS:HG2	1:E:382:ASP:HA	1.83	0.60
1:B:50:VAL:HG21	1:B:55:ILE:HD11	1.83	0.60
1:H:393:LEU:HD23	1:H:393:LEU:N	2.15	0.60
1:A:135:SER:CB	1:A:141:ALA:HB3	2.31	0.60
1:B:390:ASP:O	1:B:393:LEU:HB2	2.02	0.60
1:F:16[B]:HIS:CD2	1:F:20:LEU:HD21	2.36	0.60
1:D:409[A]:PHE:HD1	1:D:410:VAL:HG23	1.64	0.60
1:E:50:VAL:HG12	1:E:53:LYS:N	2.15	0.60
1:F:140:HIS:O	1:F:200:SER:HB3	2.00	0.60
1:G:235:THR:O	1:G:239:ILE:HG13	2.01	0.60
1:H:156:CYS:HB2	1:H:159:CYS:O	2.02	0.60
1:C:400:PRO:HB2	1:C:413:LEU:CD2	2.31	0.60
1:E:30:GLY:HA2	1:E:406:GLY:HA3	1.83	0.60
1:E:306:LEU:HD22	1:E:343:VAL:HG23	1.84	0.60
1:B:277:THR:O	1:B:281:LEU:HG	2.02	0.60
1:D:140:HIS:HA	1:D:203:ASP:OD1	2.02	0.60
1:G:367:LEU:HD22	6:G:471:HOH:O	2.01	0.60
1:A:184:GLN:HE21	1:A:185:MET:HG3	1.65	0.59
1:B:258:ASP:OD2	1:B:314:ARG:NH1	2.35	0.59
1:H:369:ARG:NH1	1:H:371:VAL:HG11	2.16	0.59
1:G:144:ARG:HD2	1:G:151:PRO:HD2	1.84	0.59
1:B:371:VAL:HB	1:B:372:PRO:HD2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:401:LEU:C	1:G:401:LEU:HD23	2.22	0.59
1:H:50:VAL:HG21	1:H:55:ILE:CD1	2.26	0.59
1:A:42:SER:HB2	1:A:45:ALA:CB	2.32	0.59
1:E:112:PRO:HA	1:E:115:GLN:HE21	1.66	0.59
1:A:72:ASN:OD1	1:A:74:PRO:HD2	2.01	0.59
1:D:40:ILE:CG1	1:D:41:LYS:H	2.16	0.59
1:A:50:VAL:O	1:A:50:VAL:HG12	2.02	0.59
1:D:196:GLY:HA3	1:D:204:PRO:O	2.02	0.59
1:A:184:GLN:NE2	6:A:517:HOH:O	2.33	0.59
1:D:42:SER:OG	1:D:45:ALA:HB2	2.03	0.59
1:F:371:VAL:HG22	1:F:372:PRO:CD	2.30	0.59
1:E:376:ALA:HB1	1:E:403:MET:HE1	1.85	0.59
1:H:212:GLU:CB	1:H:216[B]:ARG:HH21	2.16	0.59
1:A:349:VAL:O	1:A:352:SER:HB2	2.03	0.59
1:B:111:TYR:O	1:B:115:GLN:HG2	2.03	0.59
1:E:67:VAL:HG23	1:E:165:LEU:HD21	1.85	0.59
1:G:331:ARG:HH11	1:G:332:LEU:HD21	1.68	0.59
1:G:389:VAL:HG22	1:G:392:LEU:HD12	1.85	0.59
1:F:376:ALA:HB1	1:F:403:MET:HE3	1.83	0.58
1:G:2:THR:HG22	1:G:3:THR:N	2.13	0.58
1:E:19:LEU:CD1	1:E:384:ASN:ND2	2.66	0.58
1:F:376:ALA:HB3	1:F:406:GLY:CA	2.33	0.58
1:A:196:GLY:HA3	1:A:204:PRO:O	2.03	0.58
1:C:135:SER:HB3	1:C:141:ALA:HB3	1.85	0.58
1:G:367:LEU:CD2	6:G:471:HOH:O	2.51	0.58
1:B:140:HIS:O	1:B:200:SER:OG	2.21	0.58
1:C:27:ILE:CD1	1:C:32:ILE:HD13	2.33	0.58
1:H:191:KCX:OQ1	1:H:232:HIS:HB2	2.03	0.58
1:H:291:PRO:O	1:H:295:ILE:HG13	2.03	0.58
1:C:12:LEU:C	1:C:12:LEU:CD2	2.70	0.58
1:C:140:HIS:O	1:C:200:SER:HB3	2.03	0.58
1:C:407[B]:ARG:HB3	1:C:407[B]:ARG:CZ	2.34	0.58
1:F:276:VAL:HG12	1:F:325:LEU:HD21	1.85	0.58
1:A:154:SER:HB2	1:A:155:PRO:HD2	1.84	0.58
1:A:7[A]:ARG:HG3	1:A:24:GLU:OE1	2.04	0.58
1:B:53:LYS:HG2	1:B:382:ASP:HA	1.85	0.58
1:E:114:LYS:NZ	6:E:478:HOH:O	2.35	0.58
1:D:176:ARG:O	1:D:180:ARG:HG3	2.03	0.58
1:E:3:THR:CG2	1:E:26:LEU:HD11	2.33	0.58
1:H:56:MET:HB2	1:H:57:PRO:HD2	1.86	0.58
1:D:349:VAL:HG23	1:D:350:ILE:HD12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:LYS:HE2	1:F:387:LYS:HA	1.85	0.57
1:H:366:LYS:HA	1:H:374:ALA:HA	1.86	0.57
1:D:111:TYR:O	1:D:115:GLN:HG2	2.04	0.57
1:F:307:HIS:CD2	1:F:311:ILE:HD11	2.38	0.57
1:G:278:TYR:CE1	1:G:301:VAL:HG11	2.39	0.57
1:G:126:ARG:NH2	1:G:405:ASP:OD2	2.35	0.57
1:A:225:ARG:NH2	1:C:204:PRO:HD3	2.18	0.57
1:B:204:PRO:HD2	1:B:207:VAL:HG21	1.87	0.57
1:G:135:SER:CB	1:G:141:ALA:HB3	2.33	0.57
1:D:390:ASP:HA	1:D:393:LEU:HD22	1.85	0.57
1:H:140:HIS:HA	1:H:203:ASP:OD1	2.05	0.57
1:A:209:GLY:O	1:A:210:TYR:HB2	2.05	0.57
1:E:87:ARG:HG3	1:F:121:LEU:HD11	1.86	0.57
1:H:154:SER:HB3	1:H:157:GLY:H	1.69	0.57
1:D:384:ASN:HD22	1:D:387:LYS:HG3	1.70	0.57
1:E:124:GLY:O	1:E:404[A]:LYS:HE2	2.05	0.57
1:G:389:VAL:HG13	1:G:389:VAL:O	2.04	0.57
1:G:50:VAL:HG12	1:G:53:LYS:H	1.68	0.57
1:E:27:ILE:HD12	1:E:32:ILE:HD13	1.86	0.57
1:D:40:ILE:CG1	1:D:41:LYS:N	2.68	0.56
1:E:31:PHE:HD1	1:E:373:GLY:O	1.88	0.56
1:G:7:ARG:CD	1:G:24:GLU:OE1	2.52	0.56
1:E:135:SER:HB3	1:E:141:ALA:HB3	1.86	0.56
1:G:123:GLU:OE2	1:G:409[B]:PHE:HE1	1.88	0.56
1:C:95:MET:HE3	1:C:103:VAL:HG11	1.87	0.56
1:F:15:ASP:OD1	1:F:369:ARG:NH2	2.39	0.56
1:C:5:LEU:HD23	1:C:6:PHE:N	2.19	0.56
1:B:235:THR:HB	1:B:236:PRO:HD2	1.88	0.56
1:E:270:TYR:CE1	1:E:318:LYS:HE2	2.40	0.56
1:F:71:PHE:CE1	1:F:328:GLU:HG2	2.39	0.56
1:B:71:PHE:HE1	1:B:328:GLU:HG2	1.70	0.56
1:C:384:ASN:ND2	1:C:387:LYS:HG3	2.21	0.55
1:F:95:MET:HE3	1:F:103:VAL:HG11	1.86	0.55
1:C:31:PHE:HB2	1:C:33:ARG:NH2	2.21	0.55
1:F:337:PHE:HB3	1:F:389:VAL:HG13	1.89	0.55
1:G:50:VAL:HG12	1:G:53:LYS:N	2.21	0.55
1:C:154:SER:HB2	1:C:155:PRO:HD2	1.87	0.55
1:B:369:ARG:NH2	1:B:371:VAL:CG1	2.62	0.55
1:D:323:THR:HG21	1:D:333:GLN:HG3	1.88	0.55
1:E:286:GLU:CG	1:E:295:ILE:HD13	2.25	0.55
1:H:327:GLY:O	1:H:330:GLN:HG3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:C	1:A:27:ILE:HD12	2.27	0.55
1:E:15:ASP:OD2	1:E:16:HIS:CE1	2.60	0.55
1:E:63:HIS:CD2	1:E:324:ASP:OD1	2.59	0.55
1:G:196:GLY:HA3	1:G:204:PRO:O	2.07	0.55
1:G:25:ILE:HD12	1:G:55:ILE:HG21	1.88	0.55
1:H:19:LEU:HD12	1:H:386:LEU:HD12	1.89	0.55
1:B:225:ARG:NH2	1:D:204:PRO:HD3	2.22	0.55
1:D:310:GLU:HG3	1:D:343:VAL:HG11	1.88	0.55
1:E:153:ASP:OD2	1:E:153:ASP:C	2.45	0.55
1:E:3:THR:HG23	1:E:27:ILE:O	2.06	0.55
1:E:281:LEU:HB3	1:E:298:ILE:CD1	2.36	0.55
1:B:284:GLU:O	1:B:288:TYR:HD2	1.90	0.55
1:H:390:ASP:HA	1:H:393:LEU:HG	1.88	0.55
1:G:4:PHE:O	1:G:26:LEU:HD12	2.07	0.55
1:H:385:PRO:HA	1:H:388:SER:O	2.07	0.55
1:A:98:ARG:NH1	1:A:395:GLN:OE1	2.35	0.55
1:B:203:ASP:O	1:B:297:LYS:NZ	2.31	0.55
1:C:3:THR:HB	1:C:44:ASN:O	2.07	0.55
1:C:123:GLU:OE1	1:C:409:PHE:CE2	2.60	0.55
1:F:380:VAL:O	1:F:400:PRO:CD	2.49	0.55
1:F:306:LEU:HG	1:F:343:VAL:HG21	1.89	0.54
1:H:19:LEU:HD13	1:H:384:ASN:HD22	1.72	0.54
1:D:244[B]:ARG:NH2	3:D:428:SO4:O2	2.39	0.54
1:G:89:VAL:HB	1:G:90:PRO:CD	2.36	0.54
1:E:24:GLU:OE2	1:E:39:PRO:HA	2.07	0.54
1:H:200:SER:HB2	1:H:203:ASP:OD2	2.07	0.54
1:A:140:HIS:CE1	1:A:197:GLY:CA	2.76	0.54
1:B:200:SER:CB	1:B:203:ASP:OD1	2.56	0.54
1:B:200:SER:HB3	1:B:203:ASP:OD1	2.08	0.54
1:C:227:THR:HG23	1:C:228:TYR:N	2.22	0.54
1:C:2:THR:HG23	1:C:3:THR:N	2.21	0.54
1:F:368:GLY:N	6:F:500:HOH:O	2.32	0.54
1:H:176[B]:ARG:HD3	1:H:180:ARG:NH2	2.23	0.54
1:H:307:HIS:HD2	1:H:311:ILE:HG13	1.73	0.54
1:A:198:VAL:O	1:A:297:LYS:HE3	2.07	0.54
1:B:140:HIS:HA	1:B:203:ASP:OD2	2.08	0.54
1:H:5:LEU:HD12	1:H:6:PHE:N	2.23	0.54
1:A:252:HIS:ND1	1:A:274:THR:OG1	2.40	0.54
1:F:184:GLN:NE2	6:F:474:HOH:O	2.40	0.54
1:G:30:GLY:HA2	1:G:405:ASP:O	2.08	0.54
1:C:111:TYR:N	1:C:112:PRO:CD	2.70	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ILE:CD1	1:F:32:ILE:HG12	2.38	0.54
1:A:346:PRO:O	1:A:350:ILE:CD1	2.54	0.54
1:C:30:GLY:HA2	1:C:406:GLY:HA3	1.90	0.54
1:F:207:VAL:HG12	1:F:208:PHE:O	2.08	0.54
1:F:276:VAL:CG2	1:F:336:GLU:CB	2.86	0.54
1:F:337:PHE:HB3	1:F:389:VAL:CG1	2.38	0.54
1:A:27:ILE:N	1:A:27:ILE:CD1	2.71	0.53
1:H:140:HIS:ND1	1:H:200:SER:OG	2.40	0.53
1:B:156:CYS:O	1:B:157:GLY:C	2.46	0.53
1:C:140:HIS:CE1	1:C:197:GLY:HA3	2.42	0.53
1:E:176[A]:ARG:HD3	1:E:221:GLU:OE2	2.07	0.53
1:G:196:GLY:HA3	1:G:207:VAL:HG12	1.90	0.53
1:H:110:GLY:C	1:H:112:PRO:HD2	2.29	0.53
1:C:13:ASP:HA	6:C:498:HOH:O	2.07	0.53
1:C:95:MET:CE	1:C:125:PRO:HG2	2.38	0.53
1:G:110:GLY:C	1:G:112:PRO:HD2	2.29	0.53
1:C:328:GLU:H	1:C:328:GLU:CD	2.11	0.53
1:C:364:GLN:O	1:C:365:ASP:HB2	2.07	0.53
1:F:395:GLN:CA	1:F:395:GLN:OE1	2.55	0.53
1:G:321:PHE:CZ	1:G:336:GLU:HB3	2.43	0.53
1:D:166:GLY:H	4:D:429:GOL:H11	1.74	0.53
1:G:205:VAL:HG13	1:G:234:TYR:CD2	2.44	0.53
1:H:313:LYS:HD2	1:H:344:LEU:CD2	2.39	0.53
1:H:7:ARG:HG3	6:H:451:HOH:O	2.08	0.53
1:C:5:LEU:CD2	1:C:5:LEU:C	2.75	0.53
1:D:140:HIS:CE1	1:D:200:SER:HG	2.25	0.53
1:D:27:ILE:CD1	1:D:32:ILE:HD13	2.38	0.53
1:G:286:GLU:HB2	1:G:295:ILE:HD11	1.91	0.53
1:F:264:VAL:HG13	1:F:269:ALA:HB3	1.91	0.53
1:F:281:LEU:HB3	1:F:298:ILE:HD11	1.89	0.53
1:H:328:GLU:CD	1:H:328:GLU:H	2.10	0.53
1:A:115[A]:GLN:HG3	1:A:116:ALA:N	2.24	0.53
1:B:294:SER:O	1:B:298:ILE:HD12	2.08	0.53
1:D:276:VAL:CG2	1:D:336:GLU:OE2	2.56	0.53
1:D:400:PRO:HB2	1:D:413:LEU:HD21	1.91	0.53
1:F:13:ASP:OD2	1:F:16[A]:HIS:ND1	2.41	0.53
1:F:71:PHE:HE1	1:F:328:GLU:OE2	1.89	0.53
1:H:244[A]:ARG:NH2	3:H:429:SO4:O3	2.42	0.53
1:A:70:GLU:HG3	1:A:76:VAL:HG22	1.90	0.53
1:H:409:PHE:CD1	1:H:410:VAL:HG23	2.43	0.53
1:C:27:ILE:HG13	1:C:403:MET:CE	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:LEU:HD12	1:D:12:LEU:N	2.23	0.53
1:D:135:SER:CB	1:D:141:ALA:HB3	2.28	0.53
1:F:37:ASP:OD1	1:F:37:ASP:N	2.33	0.53
1:H:7:ARG:HG2	1:H:8:ASN:N	2.24	0.53
1:A:111:TYR:CD1	1:A:114[A]:LYS:HD2	2.44	0.52
1:B:199:ALA:HB3	3:B:427:SO4:O2	2.09	0.52
1:C:49:ASP:OD2	1:C:51:LYS:HG2	2.09	0.52
1:D:263:LEU:HD11	1:D:267:HIS:NE2	2.24	0.52
1:F:123:GLU:OE1	1:F:409[A]:PHE:HD2	1.91	0.52
1:H:335:ASP:O	1:H:339:ILE:HG13	2.10	0.52
1:C:349:VAL:CG2	1:C:350:ILE:HD12	2.39	0.52
1:C:400:PRO:CB	1:C:413:LEU:HD21	2.37	0.52
1:C:6:PHE:CE1	1:C:48:ILE:HD13	2.45	0.52
1:F:276:VAL:CG2	1:F:336:GLU:HA	2.40	0.52
1:E:286:GLU:O	1:E:286:GLU:OE1	2.27	0.52
1:A:72:ASN:O	1:A:76:VAL:HG23	2.10	0.52
1:D:290:LEU:C	1:D:290:LEU:CD1	2.77	0.52
1:E:103:VAL:HG22	1:E:125:PRO:HB2	1.91	0.52
1:B:408:LEU:CD1	1:B:411:ASN:HD22	2.22	0.52
1:C:82:VAL:HG23	6:C:553:HOH:O	2.08	0.52
1:D:183:LEU:HD22	1:D:225:ARG:HD3	1.92	0.52
1:D:216[A]:ARG:HG2	6:D:460:HOH:O	2.08	0.52
1:A:177:ARG:O	1:A:181:GLU:HG3	2.10	0.52
1:C:379:LEU:HD22	1:C:402:VAL:HG22	1.91	0.52
1:C:50:VAL:HG12	1:C:53:LYS:N	2.25	0.52
1:F:5:LEU:O	1:F:5:LEU:HD23	2.10	0.52
1:G:7:ARG:NE	1:G:24:GLU:OE1	2.42	0.52
1:B:199:ALA:N	3:B:427:SO4:O2	2.32	0.52
1:G:212:GLU:O	1:G:216[B]:ARG:HG3	2.09	0.52
1:H:89:VAL:HB	1:H:90:PRO:HD3	1.90	0.52
1:B:10:ALA:HB1	1:B:19:LEU:HB3	1.90	0.52
1:F:340:LEU:O	1:F:344:LEU:HB2	2.10	0.52
1:G:174:GLU:HB2	6:G:469:HOH:O	2.09	0.52
1:H:9:GLY:HA3	1:H:50:VAL:HB	1.92	0.52
1:B:408:LEU:HD13	1:B:411:ASN:ND2	2.25	0.52
1:G:170:ASP:O	1:G:174:GLU:CB	2.58	0.52
1:H:369:ARG:HH11	1:H:371:VAL:HG11	1.75	0.52
1:A:292:PRO:HA	1:A:295:ILE:HD12	1.91	0.51
1:A:331:ARG:HD3	1:A:332:LEU:HG	1.92	0.51
1:C:5:LEU:HD21	1:C:7[A]:ARG:HD3	1.91	0.51
1:D:290:LEU:HD11	1:D:294:SER:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:376:ALA:HB1	1:G:403:MET:HE3	1.84	0.51
1:C:54:THR:OG1	1:C:383:GLY:O	2.21	0.51
1:D:323:THR:HG21	1:D:333:GLN:CG	2.40	0.51
1:G:27:ILE:HG13	1:G:403:MET:HE3	1.91	0.51
1:H:12:LEU:HD23	1:H:13:ASP:N	2.24	0.51
1:H:175:VAL:O	1:H:179:VAL:HG23	2.10	0.51
1:B:389:VAL:O	1:B:389:VAL:HG13	2.11	0.51
1:F:5:LEU:C	1:F:5:LEU:HD23	2.31	0.51
1:H:53:LYS:HD2	1:H:382:ASP:OD1	2.11	0.51
1:C:156:CYS:SG	1:C:158:CYS:HB3	2.50	0.51
1:H:95:MET:HE1	1:H:125:PRO:CG	2.37	0.51
1:E:367:LEU:HD22	6:E:438:HOH:O	2.09	0.51
1:E:32:ILE:HB	1:E:371:VAL:O	2.11	0.51
1:F:290:LEU:C	1:F:290:LEU:HD13	2.30	0.51
1:H:373:GLY:N	6:H:492:HOH:O	2.44	0.51
1:A:41:LYS:HG2	1:A:41:LYS:O	2.11	0.51
1:E:71:PHE:HD1	6:E:521:HOH:O	1.94	0.51
1:H:346:PRO:O	1:H:350:ILE:HD13	2.10	0.51
1:H:408:LEU:HD13	1:H:411:ASN:HD22	1.75	0.51
1:D:263:LEU:HD11	1:D:267:HIS:CD2	2.45	0.51
1:D:71:PHE:HB3	1:D:290:LEU:HB2	1.93	0.51
1:G:274:THR:O	1:G:277:THR:HG22	2.11	0.51
1:D:387:LYS:HA	1:D:387:LYS:HE2	1.93	0.51
1:H:225:ARG:CD	6:H:483:HOH:O	2.58	0.51
1:F:286:GLU:HG2	1:F:295:ILE:HD11	1.90	0.51
1:F:71:PHE:HE1	1:F:328:GLU:CG	2.24	0.51
1:H:255:LEU:CG	1:H:301:VAL:HG12	2.41	0.51
1:H:350:ILE:O	1:H:350:ILE:CG2	2.58	0.50
1:B:135:SER:HB2	1:B:141:ALA:HB3	1.92	0.50
1:D:256:ILE:HG13	1:D:260:THR:OG1	2.11	0.50
1:E:9:GLY:CA	1:E:50:VAL:HG11	2.41	0.50
1:A:2:THR:O	1:A:2:THR:CG2	2.56	0.50
1:B:5:LEU:CD2	1:B:7:ARG:NH2	2.74	0.50
1:A:117:VAL:CG1	1:A:404[A]:LYS:HZ1	2.25	0.50
1:H:20:LEU:HB3	1:H:23:PHE:CE2	2.46	0.50
1:H:95:MET:CE	1:H:103:VAL:CG1	2.62	0.50
1:A:38:LYS:O	1:A:39:PRO:C	2.49	0.50
1:F:28:GLU:OE2	1:F:33:ARG:HG2	2.12	0.50
1:F:98:ARG:NH1	1:F:331:ARG:HA	2.27	0.50
1:B:44:ASN:CG	1:B:44:ASN:O	2.49	0.50
1:C:13:ASP:OD1	1:C:13:ASP:C	2.49	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:PRO:HB2	1:C:202:THR:HG23	1.94	0.50
1:C:27:ILE:HG13	1:C:403:MET:HE1	1.94	0.50
1:C:40:ILE:CG2	1:C:41:LYS:N	2.75	0.50
1:D:165:LEU:HB2	4:D:429:GOL:H2	1.94	0.50
1:F:61:ASP:OD1	1:F:322:GLY:HA2	2.12	0.50
1:F:292:PRO:HA	1:F:295:ILE:HD12	1.93	0.50
1:F:331:ARG:HD3	1:F:332:LEU:HD23	1.93	0.50
1:F:177:ARG:NH2	1:G:174:GLU:OE1	2.38	0.50
1:H:349:VAL:O	1:H:352:SER:HB2	2.12	0.50
1:H:68:ALA:O	1:H:330:GLN:NE2	2.45	0.50
1:A:111:TYR:N	1:A:112:PRO:CD	2.75	0.50
1:A:37:ASP:O	1:A:39:PRO:CD	2.59	0.50
1:B:297:LYS:O	1:B:300:ASP:OD2	2.30	0.50
1:D:50:VAL:HG21	1:D:55:ILE:CG1	2.42	0.50
1:E:27:ILE:N	1:E:27:ILE:HD13	2.27	0.50
1:F:27:ILE:HG13	1:F:403:MET:CE	2.41	0.50
1:F:12:LEU:HD13	1:F:56:MET:HE3	1.94	0.50
1:G:209:GLY:O	1:G:210:TYR:HB2	2.12	0.50
1:A:251:GLU:O	1:A:252:HIS:HB2	2.12	0.49
1:F:291:PRO:O	1:F:295:ILE:HG13	2.11	0.49
1:G:3:THR:HG23	1:G:28:GLU:HG2	1.93	0.49
1:A:103:VAL:HG22	1:A:125:PRO:HB2	1.94	0.49
1:D:11:LEU:HD12	1:D:12:LEU:H	1.76	0.49
1:F:258:ASP:O	1:F:262:ARG:HG3	2.13	0.49
1:F:27:ILE:HG13	1:F:403:MET:HE2	1.94	0.49
1:G:254:ASN:CG	1:G:301:VAL:HG13	2.31	0.49
1:G:331:ARG:HD3	1:G:332:LEU:HD23	1.94	0.49
1:A:25:ILE:HG23	1:A:35:VAL:HG22	1.94	0.49
1:C:401:LEU:HD23	1:C:401:LEU:C	2.33	0.49
1:D:244[B]:ARG:NE	3:D:428:SO4:O2	2.43	0.49
1:E:236:PRO:HD2	6:E:432:HOH:O	2.12	0.49
1:F:50:VAL:O	1:F:51:LYS:CB	2.60	0.49
1:G:30:GLY:HA2	1:G:406:GLY:HA3	1.94	0.49
1:H:346:PRO:HB3	1:H:385:PRO:O	2.12	0.49
1:A:79:LEU:O	1:A:161:ARG:NH2	2.46	0.49
1:C:209:GLY:O	1:C:210:TYR:HB2	2.12	0.49
1:D:50:VAL:CG2	1:D:55:ILE:HD11	2.28	0.49
1:H:255:LEU:HG	1:H:301:VAL:HG12	1.94	0.49
1:H:363:MET:HA	1:H:363:MET:CE	2.41	0.49
1:A:170:ASP:O	1:A:174:GLU:HB2	2.11	0.49
1:B:271:VAL:HG11	1:B:312:MET:SD	2.52	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:HIS:CD2	1:B:324:ASP:HB2	2.47	0.49
1:F:95:MET:HE3	1:F:103:VAL:HG21	1.94	0.49
1:H:384:ASN:O	1:H:384:ASN:OD1	2.29	0.49
1:E:281:LEU:HB3	1:E:298:ILE:HD13	1.95	0.49
1:G:71:PHE:HB3	1:G:290:LEU:HD13	1.94	0.49
1:H:239:ILE:O	1:H:243:VAL:HG23	2.12	0.49
1:C:12:LEU:HD23	1:C:13:ASP:N	2.27	0.49
1:G:61:ASP:OD1	1:G:322:GLY:HA2	2.12	0.49
1:D:3:THR:HG23	1:D:27:ILE:O	2.13	0.49
1:F:111:TYR:N	1:F:112:PRO:CD	2.75	0.49
1:F:345:SER:HB3	1:F:348:GLU:OE1	2.12	0.49
1:B:184:GLN:HG2	1:D:150:MET:SD	2.53	0.49
1:E:376:ALA:HB1	1:E:403:MET:HE3	1.95	0.48
1:G:286:GLU:HB2	1:G:295:ILE:CD1	2.43	0.48
1:A:380:VAL:HB	1:A:401:LEU:HB3	1.94	0.48
1:A:384:ASN:C	1:A:384:ASN:OD1	2.51	0.48
1:D:12:LEU:CD2	1:D:12:LEU:C	2.81	0.48
1:D:276:VAL:HG22	1:D:336:GLU:OE2	2.13	0.48
1:G:175:VAL:O	1:G:179:VAL:HG23	2.13	0.48
1:A:207:VAL:HG23	1:G:225:ARG:HA	1.95	0.48
1:A:5:LEU:HD23	1:A:5:LEU:C	2.34	0.48
1:F:204:PRO:HD2	1:F:207:VAL:CG2	2.36	0.48
1:F:368:GLY:HA2	6:F:500:HOH:O	2.12	0.48
1:G:400:PRO:HB2	1:G:413:LEU:HD13	1.94	0.48
1:H:281:LEU:HB3	1:H:298:ILE:HD13	1.94	0.48
1:H:293:GLU:HG2	1:H:294:SER:N	2.27	0.48
1:A:53:LYS:HG2	1:A:382:ASP:HA	1.95	0.48
1:B:155:PRO:HG2	1:B:156:CYS:H	1.79	0.48
1:D:30:GLY:HA2	1:D:406:GLY:HA3	1.95	0.48
1:F:332:LEU:O	1:F:333:GLN:C	2.52	0.48
1:D:156:CYS:O	1:D:157:GLY:C	2.52	0.48
1:D:376:ALA:HB1	1:D:403:MET:HE3	1.95	0.48
1:F:413:LEU:HD23	1:F:413:LEU:N	2.28	0.48
1:C:3:THR:HG22	1:C:4:PHE:N	2.29	0.48
1:G:126:ARG:HB3	1:G:126:ARG:HH11	1.79	0.48
1:C:244[A]:ARG:NH1	6:C:555:HOH:O	2.46	0.48
1:C:89:VAL:HB	1:C:90:PRO:CD	2.44	0.48
1:D:70:GLU:HA	1:D:327:GLY:CA	2.43	0.48
1:F:401:LEU:C	1:F:401:LEU:CD2	2.78	0.48
1:G:305:GLY:O	1:G:308[A]:SER:OG	2.26	0.48
1:H:19:LEU:HD13	1:H:386:LEU:HD12	1.93	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:SER:O	1:E:155:PRO:C	2.52	0.48
1:F:399:ILE:HG13	6:F:461:HOH:O	2.13	0.48
1:C:95:MET:HE1	1:C:103:VAL:HG21	1.95	0.48
1:C:123:GLU:OE1	1:C:409:PHE:HE2	1.96	0.48
1:G:300:ASP:N	1:G:300:ASP:OD2	2.46	0.48
1:H:346:PRO:CB	1:H:386:LEU:O	2.58	0.48
1:H:409:PHE:CE1	1:H:410:VAL:HG23	2.49	0.48
1:H:411:ASN:OD1	1:H:413:LEU:CB	2.62	0.48
1:C:40:ILE:HG22	1:C:41:LYS:N	2.29	0.48
1:D:14:PRO:HD2	1:D:369:ARG:HG2	1.96	0.48
1:E:64:VAL:HG11	1:E:95:MET:HE1	1.94	0.48
1:F:276:VAL:HG21	1:F:336:GLU:CB	2.41	0.48
1:H:16[B]:HIS:HE1	1:H:18:ASP:HB2	1.79	0.48
1:C:349:VAL:HG22	1:C:350:ILE:CD1	2.42	0.47
1:E:227:THR:HG23	1:E:228:TYR:N	2.29	0.47
1:D:387:LYS:CA	1:D:387:LYS:HE2	2.43	0.47
1:H:363:MET:HA	1:H:363:MET:HE2	1.95	0.47
1:H:94:ALA:HB1	1:H:98:ARG:HH12	1.79	0.47
1:C:274:THR:O	1:C:277:THR:HG22	2.14	0.47
1:B:176:ARG:NH2	6:B:491:HOH:O	2.47	0.47
1:D:190:ILE:O	1:D:230:LEU:HD23	2.15	0.47
1:F:306:LEU:HG	1:F:343:VAL:CG2	2.44	0.47
1:H:120:GLY:HA2	6:H:448:HOH:O	2.13	0.47
1:H:308:SER:O	1:H:312:MET:HG3	2.14	0.47
1:B:140:HIS:ND1	1:B:197:GLY:CA	2.58	0.47
1:F:3:THR:HG22	1:F:45:ALA:HB2	1.95	0.47
1:F:71:PHE:HB3	1:F:290:LEU:CD2	2.41	0.47
1:G:281:LEU:O	1:G:285:GLY:N	2.45	0.47
1:H:9:GLY:HA3	1:H:50:VAL:CG1	2.44	0.47
1:A:191:KCX:HD2	1:A:230:LEU:CD1	2.45	0.47
1:B:346:PRO:HD3	6:B:510:HOH:O	2.14	0.47
1:G:20:LEU:HB3	1:G:23:PHE:CE2	2.50	0.47
1:H:9:GLY:HA3	1:H:50:VAL:HG11	1.95	0.47
1:D:70:GLU:HG2	1:D:76:VAL:CG2	2.44	0.47
1:E:111:TYR:O	1:E:115:GLN:HG2	2.15	0.47
1:E:204:PRO:HD2	1:E:207:VAL:HG21	1.95	0.47
1:F:32:ILE:CD1	1:F:370:ILE:HG23	2.35	0.47
1:G:37:ASP:O	1:G:39:PRO:HD3	2.15	0.47
1:H:9:GLY:CA	1:H:50:VAL:HB	2.44	0.47
1:A:41:LYS:CG	1:A:41:LYS:O	2.63	0.47
1:C:66:VAL:HG22	1:C:109:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:HIS:CE1	1:F:106:ALA:HB3	2.50	0.47
1:F:285:GLY:O	1:F:290:LEU:CB	2.62	0.47
1:E:21[B]:GLN:CD	1:E:22:GLY:H	2.18	0.47
1:E:46:HIS:C	1:E:46:HIS:CD2	2.88	0.47
1:G:149:TYR:CE1	1:G:151:PRO:HG3	2.49	0.47
1:E:9:GLY:HA3	1:E:50:VAL:HG11	1.96	0.47
1:F:239:ILE:O	1:F:243:VAL:HG23	2.15	0.47
1:G:278:TYR:CD1	1:G:301:VAL:HG11	2.50	0.47
1:H:350:ILE:HG22	1:H:350:ILE:O	2.15	0.47
1:A:111:TYR:O	1:A:115[B]:GLN:HG3	2.15	0.47
1:B:11:LEU:HD12	1:B:12:LEU:N	2.29	0.47
1:D:111:TYR:N	1:D:112:PRO:CD	2.78	0.47
1:D:184:GLN:NE2	6:D:457:HOH:O	2.48	0.47
1:D:65:HIS:CD2	1:D:324:ASP:OD1	2.68	0.47
1:G:111:TYR:O	1:G:115:GLN:HG2	2.15	0.47
1:G:403:MET:CE	1:G:406:GLY:HA2	2.44	0.47
1:H:225:ARG:HD3	6:H:483:HOH:O	2.15	0.47
1:H:38:LYS:C	1:H:39:PRO:O	2.52	0.47
1:D:277:THR:HA	1:D:325:LEU:HD23	1.97	0.46
1:E:365:ASP:CG	1:E:369:ARG:HH21	2.16	0.46
1:G:332:LEU:O	1:G:333:GLN:C	2.53	0.46
1:G:384:ASN:OD1	1:G:386:LEU:N	2.48	0.46
1:A:50:VAL:CG1	1:A:53:LYS:HB2	2.45	0.46
1:B:89:VAL:N	1:B:90:PRO:HD2	2.30	0.46
1:E:31:PHE:CD1	1:E:373:GLY:O	2.69	0.46
1:H:16[B]:HIS:CE1	1:H:18:ASP:HB2	2.50	0.46
1:H:321:PHE:CZ	1:H:336:GLU:CB	2.93	0.46
1:H:95:MET:HE2	1:H:95:MET:HB3	1.75	0.46
1:D:73:LEU:N	1:D:74:PRO:CD	2.77	0.46
1:E:376:ALA:O	1:E:403:MET:HE3	2.15	0.46
1:F:389:VAL:O	1:F:389:VAL:CG1	2.62	0.46
1:C:4:PHE:HB2	1:C:27:ILE:HB	1.96	0.46
1:C:53:LYS:HD3	1:C:382:ASP:OD1	2.15	0.46
1:D:26:LEU:HB3	1:D:34:GLU:HB2	1.98	0.46
1:A:249:THR:HG21	1:A:360:VAL:HG13	1.98	0.46
1:D:276:VAL:HG22	1:D:336:GLU:CB	2.45	0.46
1:E:26:LEU:C	1:E:27:ILE:HD13	2.35	0.46
1:G:56:MET:HB2	1:G:57:PRO:HD2	1.98	0.46
1:A:7[A]:ARG:NH1	1:A:49:ASP:OD2	2.49	0.46
1:F:28:GLU:HB2	1:F:33:ARG:HD3	1.96	0.46
1:G:376:ALA:O	1:G:403:MET:HE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:236:PRO:HD3	1:H:255:LEU:O	2.16	0.46
1:H:41:LYS:HE2	1:H:41:LYS:HB2	1.63	0.46
1:B:214:GLU:O	1:B:218:ILE:HG13	2.16	0.46
1:C:135:SER:CB	1:C:141:ALA:HB3	2.45	0.46
1:F:294:SER:O	1:F:297:LYS:HB2	2.16	0.46
1:F:376:ALA:HB1	1:F:403:MET:CE	2.45	0.46
1:B:135:SER:CB	1:B:141:ALA:HB3	2.46	0.46
1:F:24:GLU:CD	1:F:39:PRO:HA	2.36	0.46
1:F:50:VAL:HG21	1:F:55:ILE:HG12	1.97	0.46
1:F:62:LEU:HD11	1:F:357:SER:HA	1.96	0.46
1:B:337:PHE:HB3	1:B:389:VAL:CG1	2.45	0.46
1:C:89:VAL:N	1:C:90:PRO:HD2	2.31	0.46
1:E:248:ARG:O	1:E:269:ALA:HB1	2.16	0.46
1:E:49:ASP:OD2	1:E:51:LYS:HG2	2.16	0.46
1:F:376:ALA:CB	1:F:406:GLY:CA	2.94	0.46
1:F:95:MET:CE	1:F:103:VAL:HG21	2.45	0.46
1:G:205:VAL:HG13	1:G:234:TYR:HD2	1.81	0.46
1:B:328:GLU:O	1:B:331:ARG:HG3	2.15	0.45
1:B:5:LEU:HD21	1:B:7:ARG:HH21	1.80	0.45
1:F:368:GLY:CA	6:F:500:HOH:O	2.64	0.45
1:G:380:VAL:HG12	1:G:400:PRO:HG2	1.97	0.45
1:H:12:LEU:HD23	1:H:12:LEU:C	2.36	0.45
1:B:270:TYR:CE1	1:B:318:LYS:HE2	2.50	0.45
1:C:50:VAL:HG12	1:C:53:LYS:CB	2.45	0.45
1:E:184:GLN:NE2	6:E:455:HOH:O	2.49	0.45
1:F:401:LEU:HD23	1:F:402:VAL:N	2.31	0.45
1:H:341:ALA:HB3	6:H:478:HOH:O	2.16	0.45
1:H:3:THR:HG23	1:H:28:GLU:HB3	1.97	0.45
1:F:235:THR:HB	1:F:236:PRO:HD2	1.98	0.45
1:F:345:SER:O	1:F:349:VAL:HG23	2.16	0.45
1:E:103:VAL:CG2	1:E:127:LEU:HD23	2.47	0.45
1:E:33:ARG:O	1:E:34:GLU:HG3	2.16	0.45
1:F:276:VAL:CG2	1:F:336:GLU:N	2.79	0.45
1:F:343:VAL:HG12	1:F:343:VAL:O	2.17	0.45
1:C:225:ARG:O	1:C:225:ARG:CG	2.64	0.45
1:G:50:VAL:HG11	1:G:53:LYS:O	2.16	0.45
1:G:82:VAL:O	1:G:86:LEU:HD22	2.16	0.45
1:A:58:GLY:HA3	1:A:101:THR:OG1	2.16	0.45
1:D:50:VAL:CG1	1:D:53:LYS:O	2.64	0.45
1:A:50:VAL:HG12	1:A:53:LYS:H	1.80	0.45
1:B:65:HIS:CD2	1:B:324:ASP:OD1	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASP:OD2	1:C:37:ASP:N	2.48	0.45
1:G:27:ILE:HD12	1:G:32:ILE:HD13	1.99	0.45
1:G:377:ASP:HA	1:G:403:MET:O	2.17	0.45
1:G:404:LYS:HB3	1:G:409[B]:PHE:CE2	2.51	0.45
1:C:118:GLU:HA	1:C:118:GLU:OE2	2.16	0.45
1:D:201:PRO:HB2	1:D:202:THR:HG23	1.99	0.45
1:D:38:LYS:O	1:D:39:PRO:C	2.55	0.45
1:E:366:LYS:HA	1:E:374:ALA:HA	1.99	0.45
1:E:19:LEU:HD11	1:E:384:ASN:CG	2.37	0.45
1:H:60:ILE:HA	1:H:102:THR:O	2.16	0.45
1:H:389:VAL:CG2	1:H:392:LEU:HD12	2.46	0.45
1:H:380:VAL:HG23	1:H:401:LEU:HD22	1.98	0.45
1:A:307:HIS:CD2	6:A:543:HOH:O	2.69	0.45
1:D:235:THR:O	1:D:239:ILE:HG13	2.16	0.45
1:H:191:KCX:HD2	1:H:230:LEU:CD1	2.47	0.45
1:H:292:PRO:HA	1:H:295:ILE:CG1	2.46	0.45
1:A:73:LEU:N	1:A:74:PRO:CD	2.80	0.45
1:B:28:GLU:CG	1:B:33:ARG:HE	2.30	0.45
1:B:50:VAL:O	1:B:50:VAL:HG12	2.17	0.45
1:C:176:ARG:O	1:C:180:ARG:HG3	2.17	0.45
1:C:403:MET:HE2	1:C:406:GLY:HA2	1.98	0.45
1:D:204:PRO:HG2	1:D:207:VAL:HB	1.99	0.45
1:E:111:TYR:N	1:E:112:PRO:CD	2.80	0.45
1:F:371:VAL:HG23	1:F:372:PRO:HD2	1.91	0.45
1:F:376:ALA:CB	1:F:406:GLY:HA2	2.46	0.45
1:G:230:LEU:HD23	1:G:230:LEU:H	1.80	0.45
1:H:212:GLU:CB	1:H:216[B]:ARG:NH2	2.73	0.45
1:H:251:GLU:O	1:H:252:HIS:HB2	2.16	0.45
1:H:19:LEU:CD2	1:H:384:ASN:HD22	2.28	0.45
1:E:216:ARG:HD3	6:E:509:HOH:O	2.16	0.44
1:G:126:ARG:CB	1:G:126:ARG:NH1	2.80	0.44
1:H:321:PHE:HE1	1:H:336:GLU:HG3	1.80	0.44
1:H:9:GLY:HA3	1:H:50:VAL:CB	2.47	0.44
1:A:156:CYS:SG	1:B:156:CYS:HA	2.57	0.44
1:B:337:PHE:HB3	1:B:389:VAL:HG11	1.99	0.44
1:F:364:GLN:O	1:F:365:ASP:HB2	2.17	0.44
1:G:411:ASN:C	1:G:411:ASN:OD1	2.55	0.44
1:B:389:VAL:O	1:B:389:VAL:CG1	2.65	0.44
1:B:409[A]:PHE:CE1	1:B:410:VAL:CG2	2.99	0.44
1:C:277:THR:HA	1:C:325:LEU:HD23	1.99	0.44
1:C:345:SER:O	1:C:348:GLU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ARG:HB3	1:C:369:ARG:NH2	2.32	0.44
1:C:95:MET:HE3	1:C:125:PRO:HG2	1.99	0.44
1:D:209:GLY:O	1:D:210:TYR:HB2	2.16	0.44
1:E:281:LEU:CB	1:E:298:ILE:HD13	2.47	0.44
1:E:89:VAL:N	1:E:90:PRO:HD2	2.31	0.44
1:H:343:VAL:O	1:H:344:LEU:HD23	2.17	0.44
1:A:212:GLU:O	1:A:216:ARG:HG3	2.17	0.44
1:A:387:LYS:HB3	1:A:387:LYS:HE2	1.73	0.44
1:C:215:ILE:O	1:C:219:VAL:HG23	2.17	0.44
1:C:369:ARG:HD2	1:C:371:VAL:CG1	2.47	0.44
1:D:123:GLU:HG2	1:D:409[B]:PHE:CE1	2.52	0.44
1:D:276:VAL:HG23	1:D:336:GLU:OE2	2.17	0.44
1:F:42:SER:OG	1:F:45:ALA:CB	2.65	0.44
1:H:244[A]:ARG:CZ	3:H:429:SO4:O3	2.66	0.44
1:H:69:ILE:HD12	1:H:87:ARG:CZ	2.48	0.44
1:C:369:ARG:HB3	1:C:369:ARG:HH21	1.81	0.44
1:C:378:VAL:HG12	1:C:379:LEU:N	2.32	0.44
1:G:126:ARG:HB2	1:G:126:ARG:NH1	2.32	0.44
1:C:54:THR:O	1:C:380:VAL:HA	2.18	0.44
1:E:156:CYS:HB2	1:F:158:CYS:HB3	1.99	0.44
1:F:290:LEU:CD1	1:F:290:LEU:C	2.86	0.44
1:G:126:ARG:CB	1:G:126:ARG:HH11	2.30	0.44
1:H:336:GLU:O	1:H:340:LEU:HG	2.18	0.44
1:A:404[B]:LYS:HB3	1:A:409[B]:PHE:CE2	2.53	0.44
1:D:290:LEU:HD13	1:D:291:PRO:N	2.33	0.44
1:E:135:SER:O	1:E:168:VAL:HA	2.18	0.44
1:E:244[B]:ARG:NH1	6:E:510:HOH:O	2.49	0.44
1:G:359:GLU:HA	1:G:364:GLN:OE1	2.18	0.44
1:H:380:VAL:O	1:H:400:PRO:HD2	2.18	0.44
1:A:115[A]:GLN:NE2	1:B:83:LEU:HD11	2.33	0.43
1:A:27:ILE:HG12	1:A:403:MET:CE	2.48	0.43
1:B:321:PHE:CZ	1:B:336:GLU:HB3	2.53	0.43
1:C:354:THR:OG1	1:C:355:ILE:N	2.50	0.43
1:C:44:ASN:O	1:C:44:ASN:CG	2.54	0.43
1:D:170:ASP:O	1:D:174:GLU:HB2	2.18	0.43
1:G:196:GLY:CA	1:G:207:VAL:HG12	2.48	0.43
1:H:111:TYR:N	1:H:112:PRO:HD3	2.31	0.43
1:H:411:ASN:C	1:H:413:LEU:H	2.21	0.43
1:C:140:HIS:NE2	3:C:427:SO4:O4	2.51	0.43
1:C:338:ARG:O	1:C:339:ILE:C	2.57	0.43
1:E:71:PHE:HB3	1:E:290:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:397:GLU:H	1:F:397:GLU:CD	2.20	0.43
1:A:251:GLU:O	1:A:252:HIS:CB	2.66	0.43
1:D:290:LEU:CD1	1:D:294:SER:HB2	2.49	0.43
1:F:205:VAL:HG13	1:F:234:TYR:CD2	2.53	0.43
1:F:290:LEU:HD13	1:F:291:PRO:N	2.33	0.43
1:F:404[B]:LYS:HE2	1:F:405:ASP:OD1	2.18	0.43
1:F:50:VAL:HG11	1:F:53:LYS:O	2.17	0.43
1:F:5:LEU:HA	1:F:25:ILE:O	2.18	0.43
1:F:62:LEU:HB2	1:F:321:PHE:O	2.18	0.43
1:A:114[A]:LYS:NZ	1:A:188:ASP:OD2	2.50	0.43
1:D:71:PHE:CD1	1:D:288:TYR:HB2	2.53	0.43
1:E:19:LEU:HD12	1:E:384:ASN:HD21	1.82	0.43
1:F:285:GLY:O	1:F:290:LEU:HB3	2.19	0.43
1:A:152:PRO:O	1:A:153:ASP:C	2.57	0.43
1:B:366:LYS:HD3	1:B:366:LYS:HA	1.76	0.43
1:C:313:LYS:NZ	1:C:348:GLU:OE2	2.41	0.43
1:F:50:VAL:CG1	1:F:53:LYS:HB2	2.48	0.43
1:G:376:ALA:CB	1:G:403:MET:CE	2.72	0.43
1:H:355:ILE:HG22	1:H:369:ARG:HG3	1.99	0.43
1:B:24:GLU:HB2	1:B:40:ILE:HG13	2.01	0.43
1:B:25:ILE:CD1	1:B:55:ILE:HG21	2.48	0.43
1:A:115[A]:GLN:HE21	1:B:83:LEU:HD11	1.82	0.43
1:C:270:TYR:N	1:C:270:TYR:CD2	2.87	0.43
1:F:277:THR:O	1:F:281:LEU:HG	2.18	0.43
1:F:276:VAL:HG23	1:F:336:GLU:HB2	2.00	0.43
1:A:140:HIS:CE1	1:A:200:SER:OG	2.71	0.43
1:A:14:PRO:HD2	1:A:369:ARG:HD2	2.00	0.43
1:A:10:ALA:HB1	1:A:19:LEU:HB3	1.99	0.43
1:F:364:GLN:H	1:F:364:GLN:CD	2.22	0.43
1:E:225:ARG:NH2	1:H:204:PRO:HD3	2.34	0.43
1:H:302:HIS:O	1:H:302:HIS:CD2	2.72	0.43
1:H:336:GLU:HA	1:H:336:GLU:OE2	2.18	0.43
1:A:377:ASP:HA	1:A:403:MET:O	2.18	0.43
1:F:270:TYR:N	1:F:270:TYR:CD2	2.86	0.43
1:G:73:LEU:N	1:G:74:PRO:CD	2.82	0.43
1:A:349:VAL:HG22	1:A:350:ILE:HD12	2.00	0.43
1:B:50:VAL:CG1	1:B:50:VAL:O	2.66	0.43
1:D:346:PRO:O	1:D:349:VAL:HG22	2.18	0.43
1:F:345:SER:HB3	1:F:348:GLU:CD	2.39	0.43
1:A:195:SER:HB2	6:A:456:HOH:O	2.19	0.43
1:B:201:PRO:HB2	1:B:202:THR:HG23	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:PRO:HA	1:B:295:ILE:HG12	2.01	0.43
1:B:331:ARG:H	1:B:331:ARG:HG3	1.71	0.43
1:C:111:TYR:HB3	1:C:112:PRO:HD3	2.01	0.43
1:C:116:ALA:O	1:C:121:LEU:HB2	2.19	0.43
1:E:24:GLU:OE2	1:E:40:ILE:N	2.48	0.43
1:F:30:GLY:HA2	1:F:406:GLY:CA	2.47	0.43
1:G:93:ARG:NH2	1:G:123:GLU:HG3	2.34	0.43
1:C:336:GLU:O	1:C:340:LEU:HG	2.19	0.42
1:E:281:LEU:HB3	1:E:298:ILE:HD11	2.01	0.42
1:F:189:GLN:HG3	1:F:230:LEU:HD22	2.00	0.42
1:G:204:PRO:O	1:G:207:VAL:HG12	2.19	0.42
1:G:68:ALA:O	1:G:330:GLN:NE2	2.52	0.42
1:H:110:GLY:C	1:H:112:PRO:CD	2.87	0.42
1:A:355:ILE:CG2	1:A:369:ARG:HG2	2.48	0.42
1:A:409[A]:PHE:CD1	1:A:410:VAL:HG23	2.54	0.42
1:C:19:LEU:HD11	1:C:384:ASN:CG	2.39	0.42
1:D:42:SER:OG	1:D:45:ALA:CB	2.67	0.42
1:F:110:GLY:C	1:F:112:PRO:HD2	2.39	0.42
1:F:194:ALA:O	1:F:195:SER:HB3	2.19	0.42
1:F:215:ILE:HG22	1:F:245:CYS:HB3	2.02	0.42
1:G:170:ASP:O	1:G:174:GLU:HB3	2.18	0.42
1:H:293:GLU:HG2	1:H:294:SER:H	1.84	0.42
1:D:12:LEU:HD23	1:D:13:ASP:N	2.34	0.42
1:D:71:PHE:CE1	1:D:288:TYR:HB2	2.54	0.42
1:E:202:THR:CG2	1:E:202:THR:O	2.66	0.42
1:F:71:PHE:CD1	1:F:328:GLU:OE2	2.72	0.42
1:A:307:HIS:HD2	6:A:543:HOH:O	2.02	0.42
1:B:284:GLU:CG	1:B:284:GLU:O	2.65	0.42
1:B:376:ALA:O	1:B:403:MET:HG2	2.20	0.42
1:C:13:ASP:HA	1:C:14:PRO:HD3	1.93	0.42
1:D:276:VAL:CG2	1:D:336:GLU:CB	2.81	0.42
1:F:376:ALA:HB3	1:F:406:GLY:H	1.80	0.42
1:H:63:HIS:CD2	1:H:324:ASP:HB2	2.54	0.42
1:D:132:ARG:CZ	1:D:160:VAL:HG22	2.49	0.42
1:E:219:VAL:O	1:E:223:GLN:HG3	2.20	0.42
1:F:242:ALA:O	1:F:247:VAL:HG13	2.20	0.42
1:F:89:VAL:N	1:F:90:PRO:HD2	2.34	0.42
1:H:200:SER:CB	1:H:203:ASP:OD2	2.67	0.42
1:H:251:GLU:O	1:H:252:HIS:CB	2.66	0.42
1:H:276:VAL:HG13	1:H:277:THR:N	2.35	0.42
1:B:33:ARG:HD3	1:B:33:ARG:HA	1.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HD12	1:B:55:ILE:HG21	2.01	0.42
1:C:257:ASP:C	1:C:257:ASP:OD1	2.58	0.42
1:E:222:ALA:HB1	1:E:227:THR:HG23	2.01	0.42
1:F:276:VAL:HG21	1:F:336:GLU:N	2.35	0.42
1:A:266:GLU:O	1:A:266:GLU:HG2	2.20	0.42
1:D:349:VAL:CG2	1:D:350:ILE:HD12	2.49	0.42
1:D:12:LEU:HD13	1:D:56:MET:HE3	2.01	0.42
1:B:184:GLN:HG3	1:B:185:MET:N	2.33	0.42
1:C:72:ASN:OD1	1:C:74:PRO:HD2	2.19	0.42
1:D:384:ASN:ND2	1:D:387:LYS:CG	2.82	0.42
1:G:285:GLY:O	1:G:290:LEU:HB2	2.20	0.42
1:A:191:KCX:OQ1	1:A:232:HIS:HB2	2.20	0.42
1:E:192:ILE:HG21	1:E:218:ILE:HG21	2.01	0.42
1:G:123:GLU:OE2	1:G:409[B]:PHE:CD1	2.72	0.42
1:G:280:ALA:O	1:G:284:GLU:HG2	2.20	0.42
1:B:28:GLU:HG2	1:B:33:ARG:HE	1.84	0.42
1:A:50:VAL:HG12	1:A:53:LYS:CB	2.49	0.41
1:B:63:HIS:HE1	1:B:191:KCX:OQ1	2.02	0.41
1:C:397:GLU:H	1:C:397:GLU:CD	2.16	0.41
1:E:203:ASP:OD1	1:E:203:ASP:N	2.51	0.41
1:E:32:ILE:HD12	1:E:370:ILE:HG23	2.01	0.41
1:F:111:TYR:N	1:F:112:PRO:HD2	2.35	0.41
1:G:184:GLN:HE21	1:G:185:MET:HG3	1.84	0.41
1:C:380:VAL:HB	1:C:401:LEU:HB3	2.02	0.41
1:D:345:SER:O	1:D:346:PRO:C	2.59	0.41
1:E:24:GLU:CD	1:E:39:PRO:HA	2.40	0.41
1:F:411:ASN:OD1	1:F:412:GLU:N	2.53	0.41
1:H:176[B]:ARG:HG3	1:H:221:GLU:CG	2.50	0.41
1:H:35:VAL:O	1:H:35:VAL:HG12	2.19	0.41
1:H:154:SER:HA	1:H:155:PRO:HD2	1.98	0.41
1:C:171:GLY:O	1:C:175:VAL:HG13	2.20	0.41
1:D:249:THR:HG21	1:D:360:VAL:HG13	2.03	0.41
1:D:386:LEU:HA	1:D:386:LEU:HD12	1.68	0.41
1:E:67:VAL:CG2	1:E:165:LEU:HD21	2.48	0.41
1:E:63:HIS:CD2	1:E:324:ASP:HB2	2.55	0.41
1:E:5:LEU:HD23	1:E:47:VAL:HG22	2.03	0.41
1:G:364:GLN:O	1:G:365:ASP:HB2	2.21	0.41
1:A:23:PHE:HB2	6:A:491:HOH:O	2.20	0.41
1:B:71:PHE:CE1	1:B:328:GLU:HG2	2.53	0.41
1:E:377:ASP:HA	1:E:403:MET:O	2.20	0.41
1:E:158:CYS:HB3	1:F:156:CYS:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:301:VAL:HG12	1:G:302:HIS:N	2.34	0.41
1:A:27:ILE:HG12	1:A:403:MET:HE1	2.02	0.41
1:B:203:ASP:HA	1:B:204:PRO:HD3	1.85	0.41
1:D:89:VAL:N	1:D:90:PRO:CD	2.84	0.41
1:F:197:GLY:O	1:F:297:LYS:HE3	2.19	0.41
1:F:276:VAL:HG23	1:F:336:GLU:HA	2.02	0.41
1:G:16:HIS:HA	1:G:17:PRO:HD3	1.93	0.41
1:B:195:SER:HB3	1:B:233:ALA:HA	2.02	0.41
1:B:288:TYR:CG	1:B:328:GLU:HG3	2.56	0.41
1:C:103:VAL:CG2	1:C:127:LEU:HD23	2.51	0.41
1:C:72:ASN:O	1:C:76:VAL:HG23	2.21	0.41
1:E:203:ASP:HA	1:E:204:PRO:HD3	1.87	0.41
1:F:212:GLU:HB3	1:F:216:ARG:NH1	2.35	0.41
1:F:4:PHE:O	1:F:26:LEU:HD12	2.21	0.41
1:G:27:ILE:HG13	1:G:403:MET:HE1	1.98	0.41
1:A:136:GLN:HG2	6:A:496:HOH:O	2.21	0.41
1:B:284:GLU:OE1	1:B:331:ARG:NH2	2.53	0.41
1:F:189:GLN:HG3	1:F:230:LEU:CD2	2.51	0.41
1:G:179:VAL:HG13	1:G:190:ILE:HG13	2.03	0.41
1:C:27:ILE:CD1	1:C:32:ILE:CD1	2.99	0.41
1:D:111:TYR:O	1:D:114:LYS:HB3	2.21	0.41
1:D:70:GLU:HA	1:D:327:GLY:HA3	2.03	0.41
1:F:177:ARG:O	1:F:181:GLU:HG3	2.20	0.41
1:G:11:LEU:HD23	1:G:20:LEU:HD12	2.03	0.41
1:H:73:LEU:O	1:H:74:PRO:C	2.59	0.41
1:A:334:SER:HB2	6:A:448:HOH:O	2.20	0.41
1:A:3:THR:HG22	1:A:4:PHE:N	2.36	0.41
1:B:199:ALA:CB	3:B:427:SO4:O2	2.67	0.41
1:C:200:SER:O	1:C:297:LYS:NZ	2.46	0.41
1:C:199:ALA:N	3:C:427:SO4:O1	2.44	0.41
1:D:191:KCX:OQ1	1:D:232:HIS:HB2	2.21	0.41
1:D:4:PHE:HB2	1:D:27:ILE:HB	2.03	0.41
1:E:69:ILE:HD12	1:E:87:ARG:CZ	2.50	0.41
1:F:276:VAL:HG23	1:F:336:GLU:CB	2.50	0.41
1:F:365:ASP:HB3	6:F:490:HOH:O	2.21	0.41
1:G:111:TYR:N	1:G:112:PRO:HD3	2.36	0.41
1:A:89:VAL:N	1:A:90:PRO:HD2	2.35	0.41
1:B:23:PHE:HB2	6:B:516:HOH:O	2.20	0.41
1:C:321:PHE:CZ	1:C:336:GLU:HB3	2.56	0.41
1:C:33:ARG:HD3	1:C:33:ARG:HA	1.91	0.41
1:D:34:GLU:OE2	1:D:40:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ILE:HG23	1:E:376:ALA:HB2	2.03	0.41
1:F:135:SER:CB	1:F:141:ALA:HB3	2.49	0.41
1:F:343:VAL:O	1:F:343:VAL:CG1	2.68	0.41
1:F:117:VAL:CG1	1:F:404[B]:LYS:HZ1	2.34	0.41
1:G:177:ARG:O	1:G:181:GLU:HG3	2.21	0.41
1:G:184:GLN:NE2	6:G:472:HOH:O	2.52	0.41
1:G:44:ASN:O	1:G:45:ALA:HB2	2.21	0.41
1:C:149:TYR:CE1	1:C:151:PRO:HD3	2.56	0.40
1:C:3:THR:HG22	1:C:45:ALA:HB1	2.01	0.40
1:E:103:VAL:HG23	1:E:127:LEU:HD23	2.02	0.40
1:F:132:ARG:CZ	1:F:160:VAL:HG22	2.51	0.40
1:G:170:ASP:O	1:G:174:GLU:HB2	2.20	0.40
1:C:30:GLY:CA	1:C:405:ASP:O	2.69	0.40
1:D:274:THR:HG21	1:D:324:ASP:HB2	2.02	0.40
1:G:207:VAL:HG13	1:G:207:VAL:O	2.20	0.40
1:B:207:VAL:HG22	1:H:225:ARG:HG3	2.03	0.40
1:B:70:GLU:HB2	6:B:547:HOH:O	2.22	0.40
1:D:387:LYS:HA	1:D:387:LYS:CE	2.51	0.40
1:D:77:ALA:HB2	4:D:429:GOL:H32	2.03	0.40
1:E:56:MET:HB2	1:E:57:PRO:HD2	2.02	0.40
1:E:61:ASP:C	1:E:61:ASP:OD1	2.60	0.40
1:H:19:LEU:CD1	1:H:384:ASN:HD22	2.34	0.40
1:A:184:GLN:HE21	1:A:185:MET:CG	2.34	0.40
1:A:180:ARG:NH1	1:C:170:ASP:OD1	2.50	0.40
1:C:30:GLY:HA2	1:C:405:ASP:O	2.22	0.40
1:D:310:GLU:O	1:D:314:ARG:HB2	2.21	0.40
1:E:176[A]:ARG:HH11	1:E:221:GLU:HG2	1.87	0.40
1:E:3:THR:OG1	1:E:28:GLU:HB3	2.21	0.40
1:G:189:GLN:HG3	1:G:230:LEU:HD22	2.03	0.40
1:G:196:GLY:HA2	1:G:203:ASP:OD2	2.21	0.40
1:G:4:PHE:HB2	1:G:27:ILE:HB	2.04	0.40
1:H:354:THR:OG1	1:H:355:ILE:N	2.55	0.40
1:B:135:SER:O	1:B:168:VAL:HA	2.21	0.40
1:B:87:ARG:O	1:B:90:PRO:HG2	2.22	0.40
1:C:140:HIS:HA	1:C:203:ASP:OD1	2.21	0.40
1:F:285:GLY:O	1:F:290:LEU:HB2	2.22	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	A	417/426 (98%)	395 (95%)	20 (5%)	2 (0%)	29	41
1	B	417/426 (98%)	388 (93%)	25 (6%)	4 (1%)	15	23
1	C	416/426 (98%)	392 (94%)	21 (5%)	3 (1%)	22	32
1	D	413/426 (97%)	386 (94%)	22 (5%)	5 (1%)	13	19
1	E	417/426 (98%)	391 (94%)	23 (6%)	3 (1%)	22	32
1	F	416/426 (98%)	384 (92%)	32 (8%)	0	100	100
1	G	415/426 (97%)	386 (93%)	24 (6%)	5 (1%)	13	19
1	H	415/426 (97%)	387 (93%)	26 (6%)	2 (0%)	29	41
All	All	3326/3408 (98%)	3109 (94%)	193 (6%)	24 (1%)	22	32

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	157	GLY
1	D	157	GLY
1	E	210	TYR
1	G	46[A]	HIS
1	G	46[B]	HIS
1	G	252	HIS
1	H	39	PRO
1	A	39	PRO
1	A	252	HIS
1	B	252	HIS
1	B	291	PRO
1	D	252	HIS
1	G	155	PRO
1	H	252	HIS
1	C	252	HIS
1	E	252	HIS
1	D	38	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	39	PRO
1	E	39	PRO
1	B	201	PRO
1	D	291	PRO
1	C	155	PRO
1	D	39	PRO
1	G	201	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/336 (99%)	313 (94%)	19 (6%)	20	33
1	B	332/336 (99%)	316 (95%)	16 (5%)	25	41
1	C	331/336 (98%)	323 (98%)	8 (2%)	49	68
1	D	328/336 (98%)	314 (96%)	14 (4%)	29	46
1	E	332/336 (99%)	319 (96%)	13 (4%)	32	50
1	F	331/336 (98%)	310 (94%)	21 (6%)	18	28
1	G	330/336 (98%)	315 (96%)	15 (4%)	27	44
1	H	330/336 (98%)	314 (95%)	16 (5%)	25	41
All	All	2646/2688 (98%)	2524 (95%)	122 (5%)	27	43

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	21	GLN
1	A	37	ASP
1	A	40	ILE
1	A	70	GLU
1	A	86	LEU
1	A	115[A]	GLN
1	A	115[B]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	159	CYS
1	A	160	VAL
1	A	184	GLN
1	A	230	LEU
1	A	232	HIS
1	A	331	ARG
1	A	349	VAL
1	A	352	SER
1	A	364	GLN
1	A	369	ARG
1	A	395	GLN
1	B	2	THR
1	B	42	SER
1	B	75	ARG
1	B	83	LEU
1	B	87	ARG
1	B	147	SER
1	B	158	CYS
1	B	184	GLN
1	B	230	LEU
1	B	276	VAL
1	B	300	ASP
1	B	313	LYS
1	B	338	ARG
1	B	364	GLN
1	B	393	LEU
1	B	395	GLN
1	C	41	LYS
1	C	86	LEU
1	C	135	SER
1	C	230	LEU
1	C	276	VAL
1	C	300	ASP
1	C	301	VAL
1	C	349	VAL
1	D	38	LYS
1	D	122	VAL
1	D	184	GLN
1	D	200	SER
1	D	230	LEU
1	D	276	VAL
1	D	290	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	293	GLU
1	D	345	SER
1	D	364	GLN
1	D	386	LEU
1	D	389	VAL
1	D	393	LEU
1	D	395	GLN
1	E	13	ASP
1	E	21[A]	GLN
1	E	21[B]	GLN
1	E	37	ASP
1	E	46	HIS
1	E	115	GLN
1	E	230	LEU
1	E	279	ASP
1	E	286	GLU
1	E	293	GLU
1	E	338	ARG
1	E	364	GLN
1	E	393	LEU
1	F	2	THR
1	F	15	ASP
1	F	33	ARG
1	F	37	ASP
1	F	41	LYS
1	F	184	GLN
1	F	200	SER
1	F	230	LEU
1	F	247	VAL
1	F	249	THR
1	F	270	TYR
1	F	290	LEU
1	F	294	SER
1	F	297	LYS
1	F	328	GLU
1	F	331	ARG
1	F	381	VAL
1	F	393	LEU
1	F	395	GLN
1	F	403	MET
1	F	410	VAL
1	G	86	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	93	ARG
1	G	156	CYS
1	G	184	GLN
1	G	195	SER
1	G	230	LEU
1	G	286	GLU
1	G	300	ASP
1	G	328	GLU
1	G	331	ARG
1	G	364	GLN
1	G	389	VAL
1	G	395	GLN
1	G	410	VAL
1	G	412	GLU
1	H	15	ASP
1	H	41	LYS
1	H	53	LYS
1	H	93	ARG
1	H	122	VAL
1	H	153	ASP
1	H	154	SER
1	H	230	LEU
1	H	258	ASP
1	H	283	SER
1	H	293	GLU
1	H	300	ASP
1	H	331	ARG
1	H	352	SER
1	H	364	GLN
1	H	384	ASN

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

Mol	Chain	Res	Type
1	A	46	HIS
1	A	184	GLN
1	B	184	GLN
1	B	411	ASN
1	C	44	ASN
1	E	46	HIS
1	E	115	GLN
1	E	184	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	115	GLN
1	F	184	GLN
1	G	16	HIS
1	G	184	GLN
1	H	184	GLN
1	H	302	HIS
1	H	307	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	H	191	1,2	7,11,12	0.77	0	4,12,14	1.28	1 (25%)
1	KCX	C	191	1,2	7,11,12	0.31	0	4,12,14	1.52	1 (25%)
1	KCX	D	191	1,2	7,11,12	0.71	0	4,12,14	1.21	1 (25%)
1	KCX	A	191	1,2	7,11,12	0.79	0	4,12,14	1.13	1 (25%)
1	KCX	B	191	1,2	7,11,12	0.76	0	4,12,14	0.94	0
1	KCX	G	191	1,2	7,11,12	0.76	0	4,12,14	1.01	0
1	KCX	E	191	1,2	7,11,12	0.75	0	4,12,14	0.99	0
1	KCX	F	191	1,2	7,11,12	0.62	0	4,12,14	1.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	H	191	1,2	-	0/7/10/12	-
1	KCX	C	191	1,2	-	1/7/10/12	-
1	KCX	D	191	1,2	-	0/7/10/12	-
1	KCX	A	191	1,2	-	1/7/10/12	-
1	KCX	B	191	1,2	-	0/7/10/12	-
1	KCX	G	191	1,2	-	0/7/10/12	-
1	KCX	E	191	1,2	-	0/7/10/12	-
1	KCX	F	191	1,2	-	0/7/10/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	KCX	CE-NZ-CX	-2.76	118.28	122.95
1	H	191	KCX	CE-NZ-CX	-2.35	118.96	122.95
1	D	191	KCX	CE-NZ-CX	-2.16	119.30	122.95
1	A	191	KCX	CE-NZ-CX	-2.03	119.51	122.95

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	191	KCX	CG-CD-CE-NZ
1	A	191	KCX	CG-CD-CE-NZ

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	191	KCX	2	0
1	D	191	KCX	1	0
1	A	191	KCX	2	0
1	B	191	KCX	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 33 ligands modelled in this entry, 16 are monoatomic - leaving 17 for Mogul analysis.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CO3	G	428	-	0,3,3	0.00	-	0,3,3	0.00	-
5	CO3	F	427	-	0,3,3	0.00	-	0,3,3	0.00	-
3	SO4	A	428	-	4,4,4	0.15	0	6,6,6	0.14	0
3	SO4	H	429	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	D	427	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	H	427	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	427	-	4,4,4	0.15	0	6,6,6	0.17	0
3	SO4	H	428	-	4,4,4	0.12	0	6,6,6	0.08	0
3	SO4	A	427	-	4,4,4	0.14	0	6,6,6	0.12	0
4	GOL	D	429	-	5,5,5	0.37	0	5,5,5	0.16	0
3	SO4	D	428	-	4,4,4	0.14	0	6,6,6	0.09	0
4	GOL	C	428	-	5,5,5	0.31	0	5,5,5	0.41	0
3	SO4	B	428	-	4,4,4	0.13	0	6,6,6	0.24	0
3	SO4	G	427	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	E	427	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	E	428	-	4,4,4	0.18	0	6,6,6	0.09	0
3	SO4	C	427	-	4,4,4	0.15	0	6,6,6	0.16	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	428	-	-	3/4/4/4	-
4	GOL	D	429	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	428	GOL	O1-C1-C2-C3
4	D	429	GOL	O1-C1-C2-C3
4	D	429	GOL	C1-C2-C3-O3
4	D	429	GOL	O1-C1-C2-O2
4	C	428	GOL	O1-C1-C2-O2
4	D	429	GOL	O2-C2-C3-O3
4	C	428	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	429	SO4	3	0
3	H	427	SO4	1	0
3	B	427	SO4	3	0
4	D	429	GOL	3	0
3	D	428	SO4	2	0
4	C	428	GOL	1	0
3	C	427	SO4	2	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](#)

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, 95th 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	A	413/426 (96%)	0.04	3 (0%) 87 86	40, 58, 96, 119	0
1	B	412/426 (96%)	0.24	24 (5%) 23 22	40, 54, 108, 136	0
1	C	412/426 (96%)	0.24	20 (4%) 29 28	39, 58, 100, 123	0
1	D	412/426 (96%)	0.17	14 (3%) 45 44	43, 63, 105, 123	0
1	E	412/426 (96%)	0.29	30 (7%) 15 13	45, 61, 109, 132	0
1	F	412/426 (96%)	0.40	37 (8%) 9 8	42, 66, 119, 132	0
1	G	412/426 (96%)	0.18	17 (4%) 37 36	41, 66, 112, 129	0
1	H	412/426 (96%)	0.42	37 (8%) 9 8	44, 72, 116, 133	0
All	All	3297/3408 (96%)	0.25	182 (5%) 25 24	39, 62, 110, 136	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	298	ILE	9.8
1	B	294	SER	7.3
1	F	294	SER	6.7
1	C	42	SER	6.3
1	B	199	ALA	6.1
1	H	44	ASN	6.1
1	H	42	SER	5.8
1	H	55	ILE	5.6
1	B	200	SER	5.5
1	B	43	SER	5.2
1	B	293	GLU	5.2
1	E	47	VAL	5.1
1	H	52	GLY	5.0
1	C	43	SER	4.8
1	C	6	PHE	4.8
1	E	291	PRO	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	5	LEU	4.7
1	H	43	SER	4.7
1	F	295	ILE	4.5
1	C	55	ILE	4.4
1	B	27	ILE	4.4
1	H	25	ILE	4.3
1	H	4	PHE	4.3
1	E	283	SER	4.3
1	F	291	PRO	4.2
1	D	299	ALA	4.2
1	E	40	ILE	4.2
1	F	301	VAL	4.2
1	F	296	ALA	4.1
1	C	44	ASN	4.1
1	F	293	GLU	4.1
1	H	11	LEU	4.1
1	F	198	VAL	4.0
1	H	19	LEU	4.0
1	F	290	LEU	4.0
1	E	42	SER	4.0
1	B	290	LEU	3.8
1	B	299	ALA	3.8
1	E	7	ARG	3.8
1	F	300	ASP	3.7
1	E	294	SER	3.7
1	G	200	SER	3.7
1	B	47	VAL	3.7
1	F	49	ASP	3.6
1	B	295	ILE	3.6
1	F	43	SER	3.6
1	D	284	GLU	3.5
1	E	48	ILE	3.5
1	B	198	VAL	3.5
1	F	48	ILE	3.5
1	F	413	LEU	3.4
1	F	299	ALA	3.4
1	H	28	GLU	3.4
1	H	33	ARG	3.4
1	A	156	CYS	3.4
1	E	45	ALA	3.3
1	B	291	PRO	3.3
1	C	294	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	48	ILE	3.3
1	F	302	HIS	3.3
1	G	199	ALA	3.3
1	H	32	ILE	3.3
1	E	43	SER	3.3
1	H	386	LEU	3.2
1	H	10	ALA	3.2
1	E	293	GLU	3.2
1	H	291	PRO	3.1
1	D	300	ASP	3.1
1	E	26	LEU	3.1
1	G	198	VAL	3.1
1	G	20	LEU	3.1
1	C	34	GLU	3.0
1	E	35	VAL	3.0
1	B	33	ARG	3.0
1	D	413	LEU	3.0
1	H	41	LYS	3.0
1	H	20	LEU	3.0
1	E	44	ASN	3.0
1	F	402	VAL	2.9
1	E	3	THR	2.9
1	F	400	PRO	2.9
1	C	47	VAL	2.9
1	E	41	LYS	2.9
1	A	155	PRO	2.9
1	B	201	PRO	2.9
1	E	5	LEU	2.9
1	E	288	TYR	2.9
1	G	281	LEU	2.8
1	F	288	TYR	2.8
1	H	22	GLY	2.8
1	H	36	SER	2.8
1	F	47	VAL	2.7
1	B	48	ILE	2.7
1	F	18	ASP	2.7
1	H	40	ILE	2.7
1	F	297	LYS	2.7
1	D	288	TYR	2.7
1	H	29	ASP	2.7
1	C	290	LEU	2.7
1	F	6	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	294	SER	2.6
1	H	35	VAL	2.6
1	F	280	ALA	2.6
1	G	10	ALA	2.6
1	H	3	THR	2.6
1	D	290	LEU	2.6
1	F	199	ALA	2.6
1	C	198	VAL	2.6
1	C	36	SER	2.6
1	E	25	ILE	2.6
1	F	46	HIS	2.6
1	F	285	GLY	2.6
1	G	301	VAL	2.5
1	E	290	LEU	2.5
1	C	50	VAL	2.5
1	F	408	LEU	2.5
1	H	200	SER	2.5
1	H	283	SER	2.5
1	C	295	ILE	2.5
1	B	29	ASP	2.5
1	F	381	VAL	2.5
1	H	385	PRO	2.5
1	F	281	LEU	2.5
1	F	303	GLY	2.5
1	D	291	PRO	2.4
1	B	5	LEU	2.4
1	H	34	GLU	2.4
1	G	54	THR	2.4
1	F	401	LEU	2.4
1	D	155	PRO	2.4
1	G	50	VAL	2.3
1	E	46	HIS	2.3
1	E	201	PRO	2.3
1	G	371	VAL	2.3
1	E	6	PHE	2.3
1	H	290	LEU	2.3
1	C	37	ASP	2.3
1	F	44	ASN	2.3
1	B	414	GLU	2.3
1	E	373	GLY	2.3
1	E	39	PRO	2.3
1	E	50	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	381	VAL	2.3
1	F	414	GLU	2.3
1	D	154	SER	2.3
1	H	26	LEU	2.3
1	C	4	PHE	2.2
1	C	33	ARG	2.2
1	H	414	GLU	2.2
1	E	298	ILE	2.2
1	G	295	ILE	2.2
1	H	295	ILE	2.2
1	A	409[A]	PHE	2.2
1	D	302	HIS	2.2
1	B	297	LYS	2.2
1	B	292	PRO	2.2
1	B	287	LYS	2.1
1	E	200	SER	2.2
1	C	40	ILE	2.1
1	G	6	PHE	2.1
1	B	26	LEU	2.1
1	D	301	VAL	2.1
1	B	28	GLU	2.1
1	G	11	LEU	2.1
1	E	49	ASP	2.1
1	G	27	ILE	2.1
1	F	283	SER	2.1
1	H	30	GLY	2.1
1	C	27	ILE	2.1
1	G	158	CYS	2.1
1	D	285	GLY	2.1
1	H	21	GLN	2.1
1	C	7[A]	ARG	2.1
1	H	6	PHE	2.1
1	B	30	GLY	2.1
1	F	292	PRO	2.0
1	E	2	THR	2.0
1	H	47	VAL	2.0
1	C	200	SER	2.0
1	D	293	GLU	2.0
1	G	389	VAL	2.0
1	F	25	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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	B-factors(Å ²)	Q<0.9
1	KCX	H	191	12/13	0.95	0.19	48,54,76,85	0
1	KCX	C	191	12/13	0.96	0.18	36,43,61,65	0
1	KCX	D	191	12/13	0.96	0.15	40,49,63,63	0
1	KCX	B	191	12/13	0.96	0.13	42,45,64,67	0
1	KCX	G	191	12/13	0.96	0.16	43,53,59,65	0
1	KCX	F	191	12/13	0.96	0.13	44,50,61,66	0
1	KCX	E	191	12/13	0.97	0.16	45,49,59,63	0
1	KCX	A	191	12/13	0.98	0.16	34,45,61,66	0

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, 95th 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	B-factors(Å ²)	Q<0.9
5	CO3	F	427	4/4	0.68	0.13	117,117,118,118	0
3	SO4	B	427	5/5	0.76	0.48	64,66,73,77	5
3	SO4	E	428	5/5	0.78	0.20	51,56,60,69	5
3	SO4	H	427	5/5	0.83	0.30	59,62,64,66	5
4	GOL	C	428	6/6	0.85	0.31	92,99,101,105	0
5	CO3	G	428	4/4	0.85	0.26	86,87,89,90	0
3	SO4	C	427	5/5	0.86	0.25	47,49,59,61	5
4	GOL	D	429	6/6	0.89	0.25	75,85,86,90	0
3	SO4	D	428	5/5	0.90	0.30	71,75,78,79	5
3	SO4	H	429	5/5	0.91	0.14	77,79,82,83	5
3	SO4	A	427	5/5	0.92	0.25	57,57,64,64	5
3	SO4	H	428	5/5	0.95	0.20	88,97,101,102	0
3	SO4	D	427	5/5	0.96	0.29	50,52,56,58	5
3	SO4	A	428	5/5	0.96	0.22	40,44,46,47	5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	E	427	5/5	0.96	0.17	41,45,53,53	5
2	ZN	D	426	1/1	0.97	0.13	73,73,73,73	0
3	SO4	G	427	5/5	0.97	0.17	35,38,49,49	5
3	SO4	B	428	5/5	0.97	0.24	37,42,48,49	5
2	ZN	B	426	1/1	0.98	0.11	66,66,66,66	0
2	ZN	D	425	1/1	0.98	0.11	63,63,63,63	0
2	ZN	E	426	1/1	0.99	0.11	68,68,68,68	0
2	ZN	F	425	1/1	0.99	0.09	73,73,73,73	0
2	ZN	F	426	1/1	0.99	0.08	76,76,76,76	0
2	ZN	H	426	1/1	0.99	0.10	72,72,72,72	0
2	ZN	G	426	1/1	0.99	0.08	70,70,70,70	0
2	ZN	E	425	1/1	0.99	0.10	63,63,63,63	0
2	ZN	C	426	1/1	0.99	0.10	66,66,66,66	0
2	ZN	A	425	1/1	0.99	0.14	59,59,59,59	0
2	ZN	B	425	1/1	0.99	0.09	62,62,62,62	0
2	ZN	C	425	1/1	0.99	0.11	63,63,63,63	0
2	ZN	A	426	1/1	0.99	0.16	66,66,66,66	0
2	ZN	H	425	1/1	0.99	0.10	72,72,72,72	0
2	ZN	G	425	1/1	1.00	0.10	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.