Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID	:	3S24
Title	:	Crystal structure of human mRNA guanylyltransferase
Authors	:	Das, K.; Chu, C.; Thyminski, J.R.; Bauman, J.D.; Guan, R.; Qiu, W.; Montelione, G.T.; Arnold, E.; Shatkin, A.J.
Deposited on	:	2011-05-16
Resolution	:	3.01 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
http://wwpdb.org/validation/2016/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:

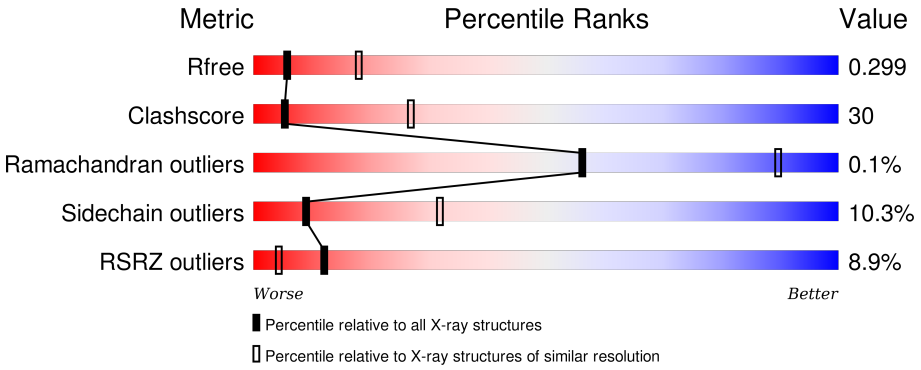
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.01 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}	91344	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	347	5% 49% 38% 8% 5%
1	B	347	13% 39% 45% 7% 9%
1	C	347	9% 44% 41% 5% 10%
1	D	347	6% 51% 39% 5% 5%
1	E	347	11% 47% 44% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	347	6% 50% 43%
1	G	347	10% 49% 40% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	5	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18387 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 mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2646	1688	457	481	20			
1	B	316	Total	C	N	O	S	0	0	0
			2561	1637	440	465	19			
1	C	314	Total	C	N	O	S	0	0	0
			2547	1628	438	462	19			
1	D	328	Total	C	N	O	S	0	0	0
			2646	1688	457	481	20			
1	E	329	Total	C	N	O	S	0	0	0
			2649	1689	456	483	21			
1	G	329	Total	C	N	O	S	0	0	0
			2651	1691	458	482	20			
1	F	333	Total	C	N	O	S	0	0	0
			2662	1698	460	484	20			

There are 56 discrepancies between the modelled and reference sequences:

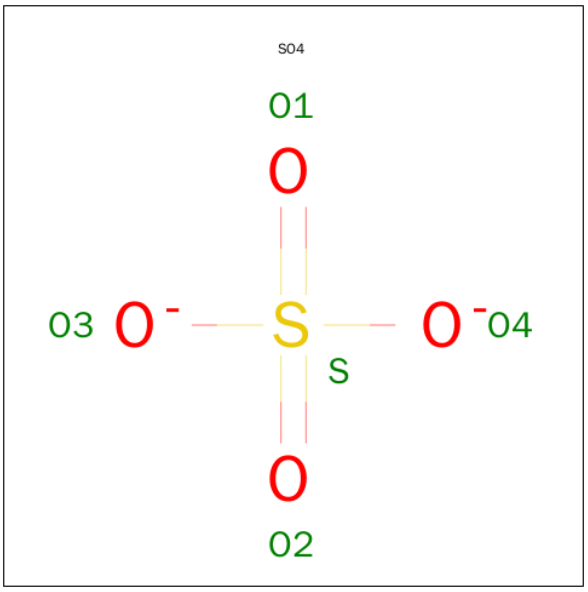
Chain	Residue	Modelled	Actual	Comment	Reference
A	568	LEU	-	EXPRESSION TAG	UNP O60942
A	569	GLU	-	EXPRESSION TAG	UNP O60942
A	570	HIS	-	EXPRESSION TAG	UNP O60942
A	571	HIS	-	EXPRESSION TAG	UNP O60942
A	572	HIS	-	EXPRESSION TAG	UNP O60942
A	573	HIS	-	EXPRESSION TAG	UNP O60942
A	574	HIS	-	EXPRESSION TAG	UNP O60942
A	575	HIS	-	EXPRESSION TAG	UNP O60942
B	568	LEU	-	EXPRESSION TAG	UNP O60942
B	569	GLU	-	EXPRESSION TAG	UNP O60942
B	570	HIS	-	EXPRESSION TAG	UNP O60942
B	571	HIS	-	EXPRESSION TAG	UNP O60942
B	572	HIS	-	EXPRESSION TAG	UNP O60942
B	573	HIS	-	EXPRESSION TAG	UNP O60942
B	574	HIS	-	EXPRESSION TAG	UNP O60942

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	575	HIS	-	EXPRESSION TAG	UNP O60942
C	568	LEU	-	EXPRESSION TAG	UNP O60942
C	569	GLU	-	EXPRESSION TAG	UNP O60942
C	570	HIS	-	EXPRESSION TAG	UNP O60942
C	571	HIS	-	EXPRESSION TAG	UNP O60942
C	572	HIS	-	EXPRESSION TAG	UNP O60942
C	573	HIS	-	EXPRESSION TAG	UNP O60942
C	574	HIS	-	EXPRESSION TAG	UNP O60942
C	575	HIS	-	EXPRESSION TAG	UNP O60942
D	568	LEU	-	EXPRESSION TAG	UNP O60942
D	569	GLU	-	EXPRESSION TAG	UNP O60942
D	570	HIS	-	EXPRESSION TAG	UNP O60942
D	571	HIS	-	EXPRESSION TAG	UNP O60942
D	572	HIS	-	EXPRESSION TAG	UNP O60942
D	573	HIS	-	EXPRESSION TAG	UNP O60942
D	574	HIS	-	EXPRESSION TAG	UNP O60942
D	575	HIS	-	EXPRESSION TAG	UNP O60942
E	568	LEU	-	EXPRESSION TAG	UNP O60942
E	569	GLU	-	EXPRESSION TAG	UNP O60942
E	570	HIS	-	EXPRESSION TAG	UNP O60942
E	571	HIS	-	EXPRESSION TAG	UNP O60942
E	572	HIS	-	EXPRESSION TAG	UNP O60942
E	573	HIS	-	EXPRESSION TAG	UNP O60942
E	574	HIS	-	EXPRESSION TAG	UNP O60942
E	575	HIS	-	EXPRESSION TAG	UNP O60942
G	568	LEU	-	EXPRESSION TAG	UNP O60942
G	569	GLU	-	EXPRESSION TAG	UNP O60942
G	570	HIS	-	EXPRESSION TAG	UNP O60942
G	571	HIS	-	EXPRESSION TAG	UNP O60942
G	572	HIS	-	EXPRESSION TAG	UNP O60942
G	573	HIS	-	EXPRESSION TAG	UNP O60942
G	574	HIS	-	EXPRESSION TAG	UNP O60942
G	575	HIS	-	EXPRESSION TAG	UNP O60942
F	568	LEU	-	EXPRESSION TAG	UNP O60942
F	569	GLU	-	EXPRESSION TAG	UNP O60942
F	570	HIS	-	EXPRESSION TAG	UNP O60942
F	571	HIS	-	EXPRESSION TAG	UNP O60942
F	572	HIS	-	EXPRESSION TAG	UNP O60942
F	573	HIS	-	EXPRESSION TAG	UNP O60942
F	574	HIS	-	EXPRESSION TAG	UNP O60942
F	575	HIS	-	EXPRESSION TAG	UNP O60942

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



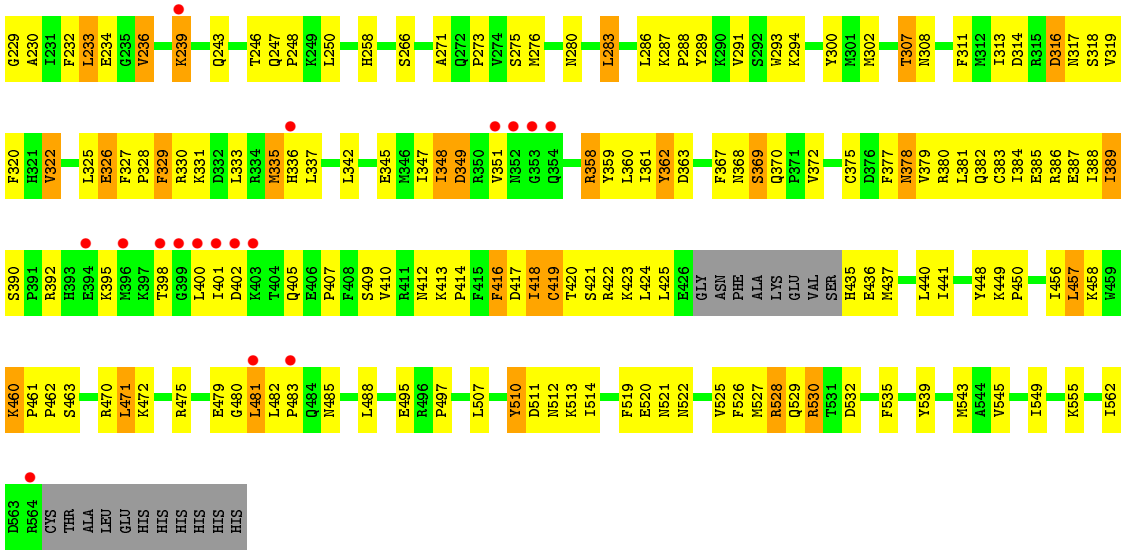
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

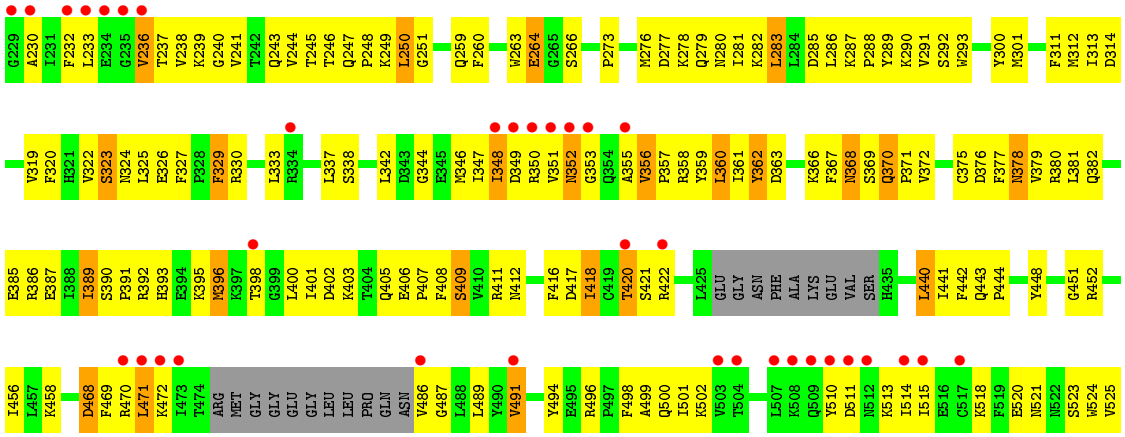
- Molecule 1: mRNA-capping enzyme

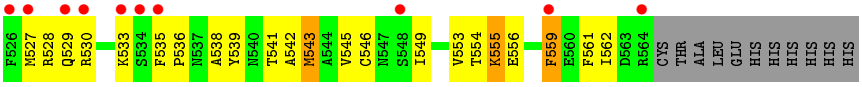
Chain A:



- Molecule 1: mRNA-capping enzyme

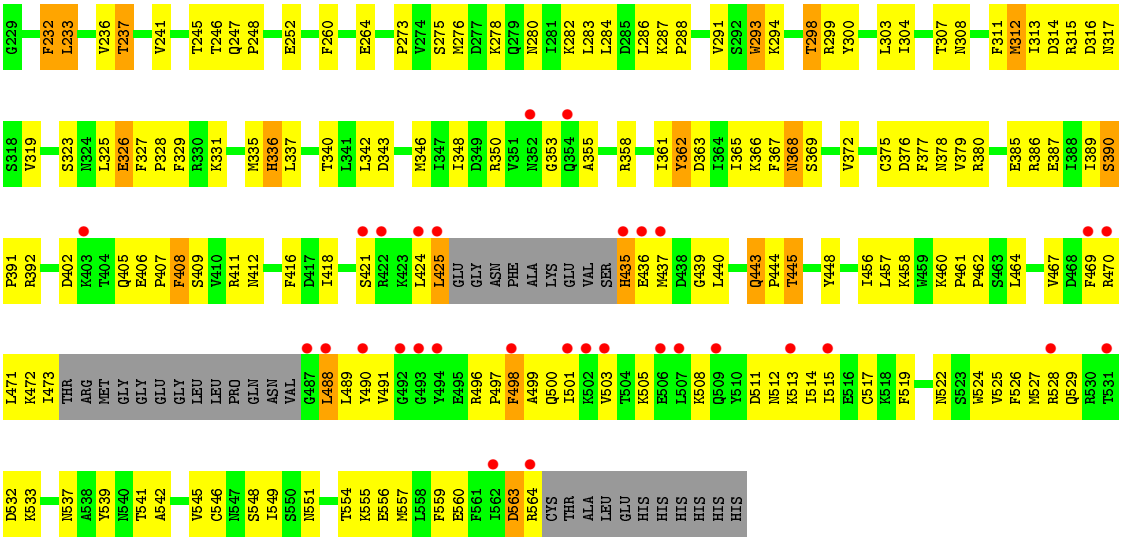
Chain B:





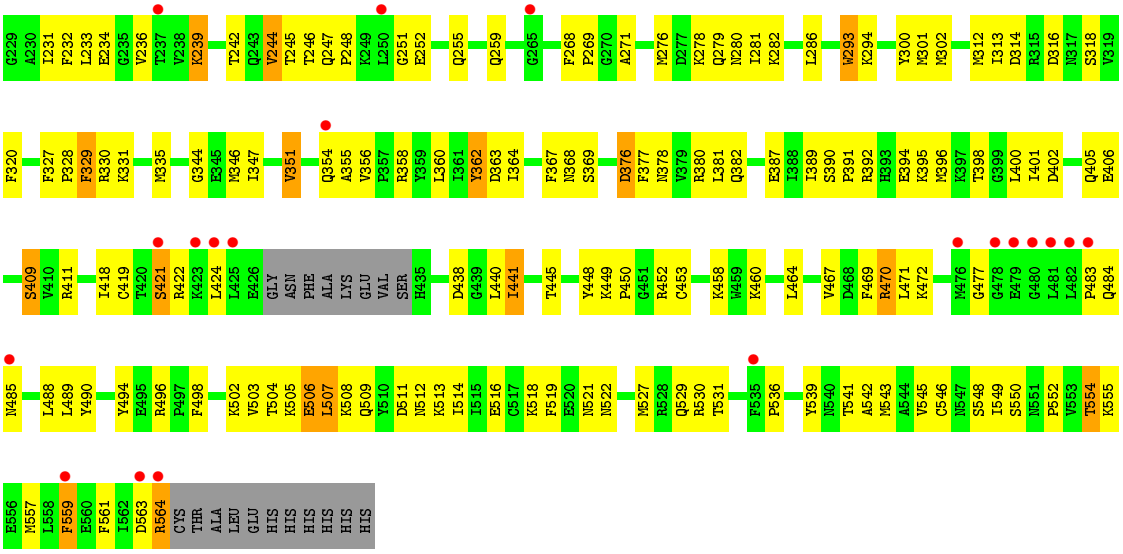
• Molecule 1: mRNA-capping enzyme

Chain C:



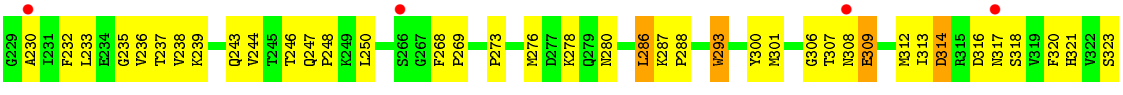
• Molecule 1: mRNA-capping enzyme

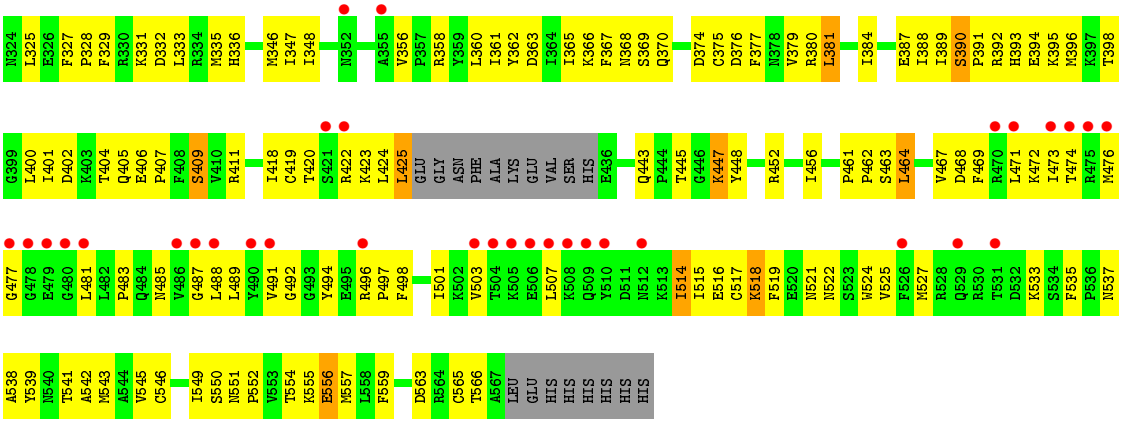
Chain D:



• Molecule 1: mRNA-capping enzyme

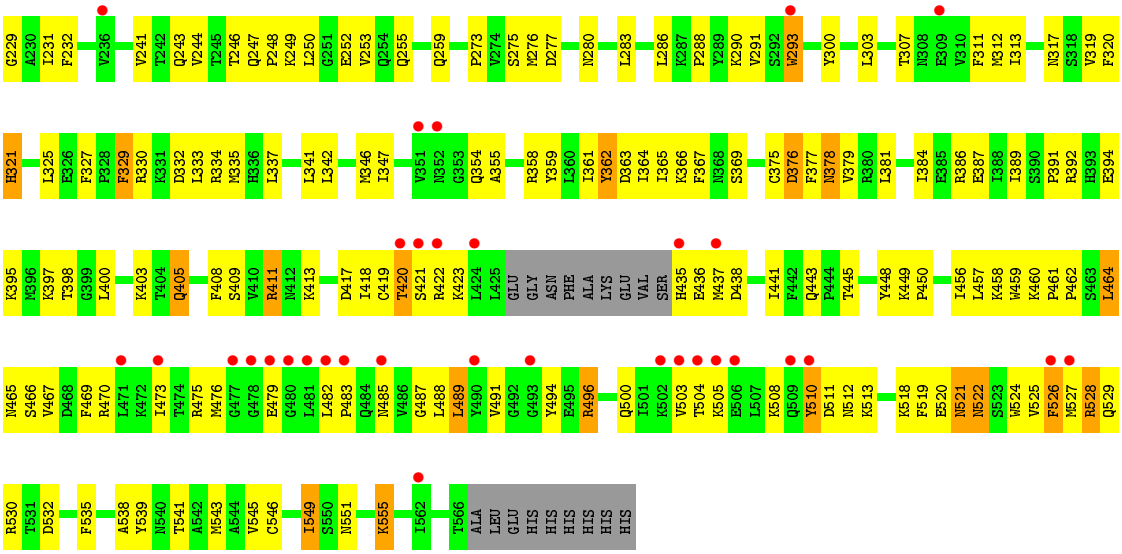
Chain E:





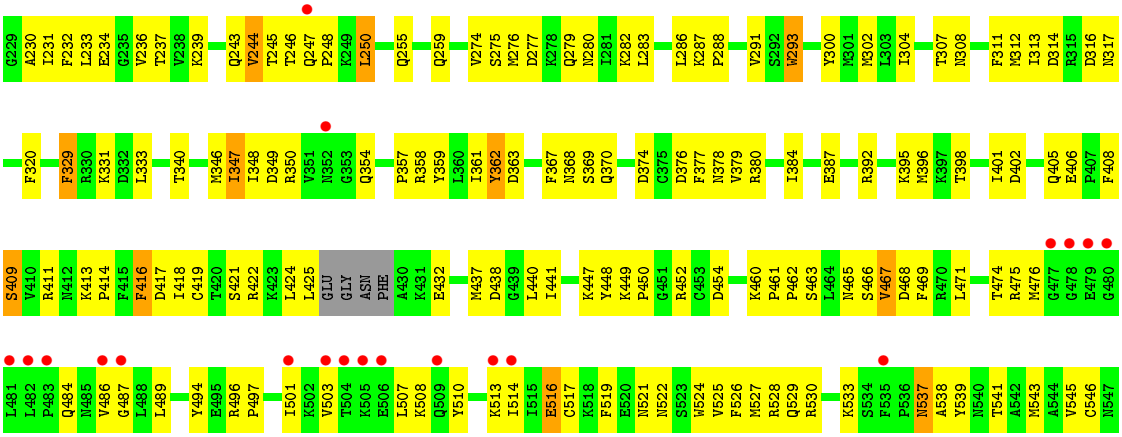
• Molecule 1: mRNA-capping enzyme

Chain G:



• Molecule 1: mRNA-capping enzyme

Chain F:




S548
I549
S550
N551
P552
V553
T554
K555
E556
M557
E560
F561
I562
D563
R564
C565
THR
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.12Å 104.66Å 149.57Å 90.00° 94.95° 90.00°	Depositor
Resolution (Å)	35.43 – 3.01 35.43 – 3.01	Depositor EDS
% Data completeness (in resolution range)	95.1 (35.43-3.01) 95.0 (35.43-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.258 , 0.296 0.254 , 0.299	Depositor DCC
R_{free} test set	2724 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	94.6	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 53399 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18387	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.56	0/2704	0.70	1/3643 (0.0%)
1	B	0.48	0/2617	0.65	2/3525 (0.1%)
1	C	0.54	0/2603	0.69	1/3505 (0.0%)
1	D	0.53	0/2704	0.68	1/3643 (0.0%)
1	E	0.55	0/2706	0.73	0/3646
1	F	0.56	0/2719	0.71	2/3665 (0.1%)
1	G	0.49	0/2709	0.66	1/3650 (0.0%)
All	All	0.53	0/18762	0.69	8/25277 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	362	TYR	CB-CA-C	6.10	122.60	110.40
1	A	362	TYR	CB-CA-C	6.01	122.41	110.40
1	C	362	TYR	CB-CA-C	5.63	121.67	110.40
1	B	362	TYR	CA-CB-CG	5.53	123.90	113.40
1	F	362	TYR	CA-CB-CG	5.30	123.48	113.40
1	D	362	TYR	CB-CA-C	5.11	120.62	110.40
1	B	362	TYR	CB-CA-C	5.06	120.52	110.40
1	G	362	TYR	CA-CB-CG	5.03	122.96	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	VAL	Peptide
1	A	480	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2646	0	2650	157	0
1	B	2561	0	2567	169	0
1	C	2547	0	2551	150	0
1	D	2646	0	2650	156	0
1	E	2649	0	2658	178	0
1	F	2662	0	2654	161	0
1	G	2651	0	2652	164	0
2	A	20	0	0	2	0
2	B	5	0	0	0	0
All	All	18387	0	18382	1106	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 30.

All (1106) 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:B:246:THR:HG22	1:B:248:PRO:HD2	1.22	1.13
1:D:239:LYS:HD3	1:D:239:LYS:H	1.17	1.08
1:C:462:PRO:HD2	1:C:555:LYS:HE3	1.37	1.06
1:A:230:ALA:HA	1:A:243:GLN:HE22	1.21	1.05
1:F:537:ASN:ND2	1:F:537:ASN:H	1.53	1.03
1:A:236:VAL:CG2	1:A:348:ILE:HD11	1.89	1.02
1:E:473:ILE:HD12	1:E:503:VAL:HG21	1.42	1.01
1:G:555:LYS:HD2	1:G:555:LYS:H	1.26	1.00
1:F:496:ARG:HB2	1:F:497:PRO:HD2	1.44	1.00
1:C:358:ARG:HG3	1:C:409:SER:HB3	1.44	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:THR:HG22	1:D:400:LEU:HD13	1.47	0.97
1:F:537:ASN:N	1:F:537:ASN:HD22	1.53	0.96
1:G:541:THR:O	1:G:545:VAL:HG23	1.67	0.94
1:E:496:ARG:HB3	1:E:497:PRO:HD2	1.49	0.94
1:A:236:VAL:HG22	1:A:348:ILE:HD11	1.49	0.93
1:A:233:LEU:HG	1:A:236:VAL:HG21	1.51	0.92
1:A:233:LEU:HG	1:A:236:VAL:CG2	1.99	0.91
1:G:504:THR:HG22	1:G:505:LYS:H	1.35	0.91
1:G:419:CYS:HA	1:G:422:ARG:HH21	1.37	0.88
1:B:546:CYS:HA	1:B:549:ILE:HG12	1.54	0.88
1:E:233:LEU:HD21	1:E:348:ILE:HD11	1.55	0.87
1:G:358:ARG:HH11	1:G:411:ARG:HE	1.23	0.87
1:C:315:ARG:HE	1:C:533:LYS:NZ	1.73	0.86
1:E:293:TRP:HD1	1:E:424:LEU:HD21	1.40	0.86
1:E:420:THR:HG23	1:E:423:LYS:HE2	1.55	0.86
1:G:504:THR:HG22	1:G:505:LYS:HG2	1.59	0.84
1:B:358:ARG:NH1	1:B:411:ARG:HH21	1.76	0.84
1:D:300:TYR:CE2	1:D:314:ASP:HB3	2.12	0.84
1:B:396:MET:CE	1:B:403:LYS:HB2	2.08	0.84
1:A:233:LEU:HB3	1:A:236:VAL:HG23	1.58	0.83
1:G:555:LYS:N	1:G:555:LYS:HD2	1.91	0.83
1:C:489:LEU:HD12	1:C:499:ALA:HB3	1.59	0.83
1:F:467:VAL:CG2	1:F:469:PHE:CE1	2.62	0.83
1:G:358:ARG:NH1	1:G:411:ARG:HE	1.77	0.82
1:E:246:THR:HG22	1:E:248:PRO:HD2	1.58	0.82
1:F:489:LEU:HD21	1:F:501:ILE:HG22	1.61	0.82
1:B:501:ILE:HD12	1:B:502:LYS:H	1.45	0.81
1:E:309:GLU:HA	1:E:309:GLU:OE1	1.81	0.81
1:A:276:MET:HA	1:A:280:ASN:HD22	1.44	0.81
1:A:327:PHE:CD1	1:A:392:ARG:HD2	2.15	0.81
1:E:314:ASP:HB3	1:E:316:ASP:H	1.44	0.80
1:A:230:ALA:HA	1:A:243:GLN:NE2	1.93	0.80
1:C:246:THR:HG22	1:C:248:PRO:HD2	1.63	0.80
1:F:402:ASP:HB3	1:F:405:GLN:HG2	1.63	0.80
1:A:230:ALA:CA	1:A:243:GLN:HE22	1.94	0.79
1:E:398:THR:OG1	1:E:400:LEU:HD13	1.82	0.79
1:B:273:PRO:HG2	1:B:458:LYS:HE3	1.65	0.78
1:C:350:ARG:NH2	1:C:353:GLY:HA2	1.97	0.78
1:B:501:ILE:HD13	1:B:524:TRP:O	1.83	0.78
1:A:372:VAL:HG12	1:A:380:ARG:HG2	1.65	0.78
1:D:358:ARG:HG3	1:D:409:SER:HB3	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:MET:HE1	1:B:403:LYS:HB2	1.66	0.78
1:G:346:MET:HE1	1:G:359:TYR:CD1	2.18	0.78
1:B:232:PHE:HB2	1:B:320:PHE:CE2	2.19	0.78
1:A:286:LEU:HD13	1:D:519:PHE:HE1	1.49	0.78
1:F:422:ARG:HH11	1:F:563:ASP:HA	1.48	0.78
1:G:435:HIS:CD2	1:G:436:GLU:H	2.00	0.77
1:C:560:GLU:HA	1:C:563:ASP:HB2	1.65	0.77
1:E:514:ILE:HD12	1:E:533:LYS:HB3	1.67	0.77
1:B:246:THR:CG2	1:B:248:PRO:HD2	2.12	0.77
1:F:246:THR:HG22	1:F:248:PRO:HD2	1.65	0.76
1:B:501:ILE:HD12	1:B:502:LYS:N	2.00	0.76
1:C:284:LEU:HD13	1:C:418:ILE:HD11	1.67	0.76
1:F:230:ALA:HB3	1:F:243:GLN:OE1	1.86	0.76
1:E:554:THR:OG1	1:E:557:MET:HB2	1.86	0.76
1:A:522:ASN:C	1:E:286:LEU:HD21	2.06	0.75
1:E:545:VAL:HG12	1:E:549:ILE:HD11	1.66	0.75
1:A:522:ASN:O	1:E:286:LEU:HD21	1.85	0.75
1:B:541:THR:O	1:B:545:VAL:HG23	1.86	0.75
1:A:539:TYR:OH	1:E:445:THR:HG21	1.86	0.75
1:D:392:ARG:O	1:D:396:MET:HG3	1.85	0.75
1:D:554:THR:HB	1:D:557:MET:H	1.51	0.75
1:F:276:MET:HA	1:F:280:ASN:HD22	1.52	0.74
1:B:236:VAL:CG1	1:B:348:ILE:HD11	2.17	0.74
1:F:291:VAL:HG11	1:F:421:SER:HB3	1.69	0.74
1:A:236:VAL:HG21	1:A:348:ILE:HD11	1.70	0.74
1:C:315:ARG:HE	1:C:533:LYS:HZ1	1.31	0.74
1:F:501:ILE:HD13	1:F:524:TRP:O	1.87	0.74
1:D:395:LYS:HB3	1:D:401:ILE:HG13	1.71	0.73
1:F:530:ARG:HH11	1:F:533:LYS:HD3	1.52	0.73
1:G:376:ASP:OD2	1:G:445:THR:HG22	1.88	0.73
1:C:276:MET:HA	1:C:280:ASN:HD22	1.53	0.73
1:G:273:PRO:HB3	1:G:456:ILE:CG2	2.18	0.72
1:A:420:THR:HG23	1:A:423:LYS:HD2	1.71	0.72
1:G:377:PHE:CE2	1:G:443:GLN:HG2	2.25	0.72
1:B:539:TYR:CE2	1:B:543:MET:HG3	2.25	0.72
1:C:329:PHE:HD2	1:C:331:LYS:H	1.34	0.72
1:D:398:THR:CG2	1:D:400:LEU:HD13	2.19	0.72
1:B:346:MET:SD	1:B:359:TYR:HB2	2.29	0.72
1:A:481:LEU:HD23	1:A:482:LEU:HD23	1.71	0.72
1:E:514:ILE:HD11	1:E:535:PHE:O	1.90	0.71
1:A:347:ILE:HD13	1:A:360:LEU:HD11	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:554:THR:H	1:F:557:MET:HE3	1.54	0.71
1:A:358:ARG:HG3	1:A:409:SER:HB3	1.73	0.71
1:E:332:ASP:OD2	1:E:335:MET:HG3	1.90	0.71
1:D:239:LYS:CD	1:D:239:LYS:H	1.95	0.71
1:A:398:THR:HG22	1:A:400:LEU:HD13	1.72	0.71
1:D:377:PHE:HD1	1:D:380:ARG:HH21	1.39	0.71
1:B:358:ARG:HG3	1:B:409:SER:HB3	1.71	0.71
1:F:346:MET:HE2	1:F:359:TYR:HD1	1.56	0.71
1:D:380:ARG:HH12	1:D:448:TYR:N	1.89	0.70
1:B:285:ASP:HB3	1:C:500:GLN:HB2	1.73	0.70
1:E:519:PHE:HE1	1:G:286:LEU:CD2	2.03	0.70
1:B:283:LEU:HA	1:B:286:LEU:HG	1.73	0.70
1:B:393:HIS:HA	1:B:396:MET:HB2	1.73	0.70
1:A:377:PHE:HD1	1:A:380:ARG:HH21	1.37	0.70
1:D:239:LYS:N	1:D:239:LYS:HD3	2.01	0.70
1:A:289:TYR:HB3	1:A:418:ILE:HD11	1.73	0.70
1:C:294:LYS:HZ2	1:C:458:LYS:HE3	1.56	0.70
1:E:420:THR:HG23	1:E:423:LYS:CE	2.20	0.70
1:F:421:SER:HA	1:F:424:LEU:HD12	1.74	0.70
1:A:247:GLN:N	1:A:248:PRO:HD2	2.07	0.70
1:G:475:ARG:HD3	1:G:483:PRO:O	1.92	0.70
1:A:335:MET:CE	1:A:336:HIS:H	2.05	0.70
1:B:489:LEU:HD21	1:B:501:ILE:HG22	1.74	0.69
1:F:422:ARG:NH1	1:F:563:ASP:HA	2.06	0.69
1:G:460:LYS:HG2	1:G:464:LEU:HD22	1.74	0.69
1:B:367:PHE:CZ	1:B:387:GLU:HB3	2.28	0.69
1:C:377:PHE:HD1	1:C:380:ARG:HH21	1.38	0.69
1:A:530:ARG:HG2	1:A:530:ARG:HH11	1.57	0.69
1:D:505:LYS:HA	1:D:508:LYS:HE3	1.75	0.69
1:G:283:LEU:HD23	1:G:286:LEU:HD22	1.75	0.69
1:C:273:PRO:HB3	1:C:456:ILE:HG22	1.75	0.69
1:F:467:VAL:HG21	1:F:469:PHE:CE1	2.28	0.68
1:E:276:MET:HA	1:E:280:ASN:HD22	1.57	0.68
1:E:496:ARG:HB3	1:E:497:PRO:CD	2.22	0.68
1:D:255:GLN:O	1:D:259:GLN:HG2	1.93	0.68
1:F:387:GLU:HA	1:F:387:GLU:OE1	1.94	0.68
1:D:469:PHE:CB	1:D:489:LEU:HB3	2.23	0.68
1:F:468:ASP:OD1	1:F:516:GLU:HB2	1.94	0.68
1:A:422:ARG:HB3	1:A:562:ILE:HG21	1.76	0.68
1:D:351:VAL:HG12	1:D:354:GLN:HB2	1.76	0.68
1:G:347:ILE:HD12	1:G:435:HIS:HB2	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:494:TYR:CD1	1:D:539:TYR:CE1	2.82	0.68
1:E:395:LYS:HB3	1:E:401:ILE:HG13	1.76	0.67
1:C:299:ARG:NH2	1:C:343:ASP:OD1	2.23	0.67
1:F:293:TRP:HB3	1:F:440:LEU:HD23	1.75	0.67
1:G:435:HIS:CG	1:G:436:GLU:H	2.09	0.67
1:G:460:LYS:HG2	1:G:464:LEU:CD2	2.23	0.67
1:G:277:ASP:H	1:G:280:ASN:HB2	1.58	0.67
1:A:367:PHE:CE1	1:A:387:GLU:HB3	2.30	0.67
1:B:538:ALA:HB3	1:B:541:THR:OG1	1.94	0.66
1:C:283:LEU:HD23	1:C:286:LEU:HD12	1.75	0.66
1:E:541:THR:O	1:E:545:VAL:HG23	1.95	0.66
1:E:392:ARG:O	1:E:396:MET:HG3	1.95	0.66
1:A:342:LEU:HD13	1:A:361:ILE:HG21	1.77	0.66
1:E:422:ARG:NH1	1:E:566:THR:HG21	2.10	0.66
1:A:349:ASP:OD2	1:A:358:ARG:NH1	2.29	0.66
1:D:471:LEU:HD12	1:D:472:LYS:N	2.11	0.66
1:G:398:THR:O	1:G:400:LEU:HD12	1.95	0.66
1:B:358:ARG:HG3	1:B:409:SER:CB	2.25	0.66
1:D:494:TYR:CD1	1:D:539:TYR:CD1	2.84	0.66
1:E:471:LEU:HB2	1:E:515:ILE:HD13	1.78	0.66
1:E:329:PHE:CE2	1:E:331:LYS:HB2	2.31	0.66
1:B:236:VAL:HG22	1:B:237:THR:H	1.61	0.66
1:B:230:ALA:HB1	1:B:243:GLN:OE1	1.95	0.66
1:A:545:VAL:O	1:A:549:ILE:HG23	1.95	0.66
1:B:489:LEU:HD21	1:B:501:ILE:CG2	2.26	0.65
1:E:393:HIS:HA	1:E:396:MET:HE2	1.77	0.65
1:B:396:MET:HG2	1:B:401:ILE:CG2	2.25	0.65
1:G:435:HIS:CG	1:G:436:GLU:N	2.65	0.65
1:D:494:TYR:HE2	1:D:496:ARG:HB2	1.60	0.65
1:B:350:ARG:HH21	1:B:353:GLY:HA2	1.60	0.65
1:G:346:MET:HE1	1:G:359:TYR:HB2	1.77	0.65
1:A:422:ARG:HB3	1:A:562:ILE:CG2	2.27	0.65
1:A:520:GLU:HG3	1:A:521:ASN:ND2	2.11	0.65
1:D:376:ASP:OD2	1:D:445:THR:HG22	1.97	0.65
1:F:467:VAL:HG12	1:F:545:VAL:HG21	1.78	0.65
1:D:504:THR:HG22	1:D:507:LEU:HB2	1.79	0.65
1:A:229:GLY:N	1:A:318:SER:HG	1.94	0.65
1:B:358:ARG:HH11	1:B:411:ARG:HH21	1.45	0.65
1:C:376:ASP:OD2	1:C:445:THR:HG22	1.97	0.65
1:A:335:MET:HE2	1:A:336:HIS:H	1.60	0.65
1:E:327:PHE:CD1	1:E:392:ARG:HD2	2.32	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:TYR:CD1	1:E:539:TYR:CE1	2.84	0.65
1:D:469:PHE:CG	1:D:489:LEU:HB3	2.31	0.65
1:C:503:VAL:HG12	1:C:508:LYS:HE3	1.77	0.65
1:B:291:VAL:HG21	1:B:440:LEU:HD13	1.79	0.65
1:C:491:VAL:HG21	1:C:539:TYR:HA	1.79	0.65
1:C:299:ARG:HH21	1:C:343:ASP:CG	1.99	0.64
1:A:368:ASN:O	1:A:369:SER:HB2	1.97	0.64
1:A:471:LEU:HD12	1:A:472:LYS:N	2.12	0.64
1:A:232:PHE:HB2	1:A:320:PHE:CE2	2.31	0.64
1:F:312:MET:HE3	1:F:346:MET:CE	2.27	0.64
1:E:293:TRP:CD1	1:E:424:LEU:HD21	2.29	0.64
1:E:420:THR:O	1:E:420:THR:HG22	1.98	0.64
1:B:327:PHE:CD1	1:B:392:ARG:HD2	2.32	0.64
1:G:403:LYS:NZ	1:G:411:ARG:NH2	2.45	0.64
1:F:541:THR:O	1:F:545:VAL:HG23	1.96	0.64
1:G:519:PHE:HB2	1:G:524:TRP:CZ3	2.33	0.64
1:F:467:VAL:CG2	1:F:469:PHE:CZ	2.80	0.64
1:B:232:PHE:CD1	1:B:241:VAL:HG11	2.33	0.63
1:A:294:LYS:HE3	1:A:345:GLU:OE1	1.98	0.63
1:A:519:PHE:CD2	1:A:549:ILE:HD12	2.33	0.63
1:C:313:ILE:HD12	1:C:313:ILE:N	2.12	0.63
1:G:538:ALA:HB3	1:G:541:THR:OG1	1.96	0.63
1:D:351:VAL:CG1	1:D:354:GLN:HB2	2.28	0.63
1:F:358:ARG:CG	1:F:409:SER:HB3	2.28	0.63
1:B:358:ARG:HD3	1:B:411:ARG:HE	1.64	0.63
1:E:278:LYS:HE3	1:E:552:PRO:O	1.98	0.63
1:C:501:ILE:HD13	1:C:524:TRP:O	1.98	0.63
1:C:335:MET:CE	1:C:335:MET:HA	2.29	0.63
1:F:233:LEU:HD22	1:F:346:MET:HG3	1.79	0.63
1:A:246:THR:HG22	1:A:248:PRO:HD2	1.81	0.63
1:E:463:SER:HB2	1:E:464:LEU:HD23	1.81	0.63
1:D:441:ILE:HD12	1:D:458:LYS:HB3	1.79	0.63
1:D:358:ARG:HD3	1:D:411:ARG:HD2	1.80	0.63
1:A:424:LEU:HD13	1:A:440:LEU:HD21	1.79	0.63
1:C:380:ARG:HH12	1:C:448:TYR:N	1.97	0.62
1:B:347:ILE:HD13	1:B:360:LEU:HD21	1.80	0.62
1:C:286:LEU:HD11	1:F:522:ASN:O	1.99	0.62
1:C:555:LYS:HB2	1:C:556:GLU:OE1	1.98	0.62
1:F:246:THR:C	1:F:248:PRO:HD2	2.19	0.62
1:D:378:ASN:O	1:D:382:GLN:HG3	1.99	0.62
1:E:425:LEU:HD11	1:E:559:PHE:HE1	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:MET:HG3	1:B:528:ARG:H	1.65	0.62
1:A:380:ARG:HH12	1:A:448:TYR:N	1.97	0.62
1:B:286:LEU:HD11	1:C:522:ASN:C	2.20	0.62
1:G:333:LEU:HD11	1:G:394:GLU:HG2	1.81	0.62
1:E:358:ARG:HH11	1:E:411:ARG:CZ	2.13	0.62
1:G:555:LYS:CD	1:G:555:LYS:H	2.08	0.62
1:F:469:PHE:CD2	1:F:489:LEU:HB3	2.34	0.62
1:E:522:ASN:C	1:G:286:LEU:HD21	2.21	0.62
1:C:236:VAL:CG1	1:C:237:THR:N	2.63	0.62
1:C:554:THR:OG1	1:C:557:MET:HB2	1.99	0.62
1:B:333:LEU:HB3	1:B:395:LYS:HE3	1.81	0.61
1:C:498:PHE:O	1:C:498:PHE:HD2	1.83	0.61
1:A:289:TYR:CB	1:A:418:ILE:HD11	2.29	0.61
1:F:467:VAL:HG23	1:F:469:PHE:CE1	2.35	0.61
1:G:273:PRO:HB3	1:G:456:ILE:HG21	1.81	0.61
1:A:300:TYR:CE2	1:A:314:ASP:HB3	2.35	0.61
1:E:377:PHE:HD1	1:E:380:ARG:HH21	1.48	0.61
1:F:466:SER:HB2	1:F:517:CYS:O	2.00	0.61
1:E:522:ASN:HA	1:G:286:LEU:HD21	1.82	0.61
1:E:489:LEU:CD2	1:E:515:ILE:HD11	2.31	0.61
1:D:293:TRP:HD1	1:D:424:LEU:HD11	1.64	0.61
1:D:469:PHE:CD2	1:D:489:LEU:HD13	2.35	0.61
1:G:520:GLU:HG3	1:G:525:VAL:HG11	1.82	0.61
1:F:421:SER:O	1:F:424:LEU:HB2	2.00	0.61
1:A:514:ILE:HG22	1:A:530:ARG:HB3	1.81	0.61
1:A:419:CYS:O	1:A:422:ARG:HG2	2.00	0.61
1:D:363:ASP:OD1	1:D:448:TYR:HD1	1.84	0.61
1:E:464:LEU:HD23	1:E:464:LEU:N	2.16	0.61
1:G:341:LEU:HD23	1:G:365:ILE:HB	1.83	0.61
1:D:246:THR:HG22	1:D:248:PRO:HD2	1.82	0.61
1:C:246:THR:CG2	1:C:248:PRO:HD2	2.31	0.60
1:A:416:PHE:HE1	1:A:424:LEU:HD11	1.66	0.60
1:F:530:ARG:NH1	1:F:533:LYS:HD3	2.14	0.60
1:A:475:ARG:HA	1:A:485:ASN:CB	2.31	0.60
1:A:280:ASN:HB3	1:A:457:LEU:CD1	2.30	0.60
1:C:348:ILE:HG23	1:C:355:ALA:HB1	1.82	0.60
1:G:246:THR:HG22	1:G:248:PRO:CD	2.31	0.60
1:E:247:GLN:OE1	1:E:247:GLN:HA	2.01	0.60
1:F:287:LYS:HB2	1:F:288:PRO:CD	2.30	0.60
1:F:487:GLY:H	1:F:503:VAL:HG23	1.67	0.60
1:C:376:ASP:HB3	1:C:379:VAL:HG23	1.81	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:PHE:HD2	1:D:330:ARG:N	2.00	0.60
1:E:329:PHE:HE2	1:E:331:LYS:HB2	1.64	0.60
1:A:293:TRP:HB3	1:A:437:MET:SD	2.41	0.60
1:E:361:ILE:HG22	1:E:384:ILE:HD13	1.83	0.60
1:E:363:ASP:OD1	1:E:448:TYR:HD1	1.84	0.60
1:F:419:CYS:HB3	1:F:422:ARG:HH21	1.67	0.60
1:F:312:MET:CE	1:F:346:MET:HE1	2.32	0.60
1:E:358:ARG:HD3	1:E:411:ARG:CD	2.31	0.60
1:A:435:HIS:CG	1:A:436:GLU:N	2.70	0.60
1:D:470:ARG:HH21	1:D:536:PRO:HD3	1.65	0.60
1:E:519:PHE:HE1	1:G:286:LEU:HD21	1.64	0.60
1:G:334:ARG:HD3	1:F:432:GLU:CB	2.31	0.60
1:G:420:THR:HG23	1:G:423:LYS:HD2	1.84	0.60
1:B:469:PHE:CG	1:B:489:LEU:HB3	2.37	0.59
1:F:494:TYR:CD2	1:F:539:TYR:CE1	2.90	0.59
1:G:511:ASP:C	1:G:513:LYS:H	2.05	0.59
1:A:271:ALA:HB2	1:A:449:LYS:O	2.01	0.59
1:A:417:ASP:HB3	1:D:496:ARG:NH1	2.18	0.59
1:D:236:VAL:HG21	1:D:355:ALA:HB1	1.84	0.59
1:A:342:LEU:HD13	1:A:361:ILE:CG2	2.33	0.59
1:G:543:MET:HA	1:G:543:MET:CE	2.32	0.59
1:G:291:VAL:HG11	1:G:421:SER:HB3	1.83	0.59
1:D:494:TYR:CE2	1:D:496:ARG:HB2	2.38	0.59
1:B:290:LYS:HA	1:B:417:ASP:HA	1.84	0.59
1:F:329:PHE:HD2	1:F:331:LYS:H	1.49	0.59
1:G:435:HIS:CD2	1:G:436:GLU:N	2.70	0.59
1:F:363:ASP:OD1	1:F:448:TYR:HD1	1.86	0.59
1:G:403:LYS:HZ1	1:G:411:ARG:NH2	1.99	0.59
1:B:491:VAL:HG22	1:B:498:PHE:HB2	1.84	0.59
1:F:246:THR:HG22	1:F:248:PRO:CD	2.32	0.58
1:A:293:TRP:O	1:A:293:TRP:CE3	2.56	0.58
1:G:504:THR:O	1:G:508:LYS:HG3	2.04	0.58
1:E:313:ILE:HD12	1:E:313:ILE:N	2.18	0.58
1:A:316:ASP:O	1:A:317:ASN:HB2	2.03	0.58
1:D:477:GLY:HA2	1:D:483:PRO:HB3	1.85	0.58
1:G:246:THR:HG22	1:G:248:PRO:HD2	1.84	0.58
1:A:280:ASN:HB3	1:A:457:LEU:HD11	1.84	0.58
1:D:293:TRP:O	1:D:293:TRP:HE3	1.86	0.58
1:G:543:MET:HE3	1:G:543:MET:HA	1.83	0.58
1:B:417:ASP:OD2	1:B:420:THR:HG22	2.03	0.58
1:E:518:LYS:HG2	1:E:519:PHE:H	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:528:ARG:HG2	1:G:528:ARG:HH11	1.68	0.58
1:D:276:MET:HA	1:D:280:ASN:HD22	1.69	0.58
1:G:403:LYS:HZ3	1:G:411:ARG:HH22	1.52	0.58
1:F:526:PHE:HZ	1:F:529:GLN:HB2	1.69	0.58
1:A:511:ASP:O	1:A:512:ASN:HB2	2.04	0.58
1:G:400:LEU:HD12	1:G:400:LEU:N	2.18	0.58
1:E:268:PHE:CD1	1:E:269:PRO:HD2	2.38	0.58
1:C:273:PRO:HB3	1:C:456:ILE:CG2	2.34	0.58
1:D:293:TRP:HD1	1:D:424:LEU:CD1	2.16	0.58
1:A:280:ASN:O	1:A:283:LEU:HB2	2.03	0.57
1:G:494:TYR:CD2	1:G:539:TYR:CD1	2.92	0.57
1:E:316:ASP:O	1:E:317:ASN:HB2	2.05	0.57
1:D:471:LEU:HD12	1:D:472:LYS:H	1.69	0.57
1:D:268:PHE:CE1	1:D:301:MET:HG3	2.40	0.57
1:D:232:PHE:HB2	1:D:320:PHE:CE2	2.39	0.57
1:E:306:GLY:CA	1:E:309:GLU:HB2	2.35	0.57
1:G:346:MET:HE1	1:G:359:TYR:HD1	1.67	0.57
1:F:280:ASN:O	1:F:283:LEU:HD12	2.05	0.57
1:G:526:PHE:CD2	1:G:526:PHE:C	2.78	0.57
1:G:513:LYS:HB3	1:G:529:GLN:NE2	2.19	0.57
1:G:470:ARG:HH22	1:G:535:PHE:HD1	1.52	0.57
1:B:372:VAL:HG12	1:B:380:ARG:HG2	1.85	0.57
1:B:396:MET:HG2	1:B:401:ILE:HG22	1.87	0.57
1:B:469:PHE:CB	1:B:489:LEU:HB3	2.33	0.57
1:D:351:VAL:O	1:D:351:VAL:HG13	2.04	0.57
1:D:330:ARG:NH2	1:D:331:LYS:HE2	2.19	0.57
1:E:374:ASP:HA	1:E:447:LYS:HB3	1.87	0.57
1:F:462:PRO:HA	1:F:465:ASN:OD1	2.04	0.57
1:E:236:VAL:HG12	1:E:237:THR:O	2.04	0.57
1:C:546:CYS:HA	1:C:549:ILE:HG12	1.86	0.57
1:G:325:LEU:HD11	1:G:408:PHE:CE1	2.39	0.57
1:F:513:LYS:HD2	1:F:529:GLN:HE22	1.69	0.57
1:B:539:TYR:CD2	1:B:539:TYR:C	2.77	0.57
1:C:236:VAL:HG12	1:C:237:THR:N	2.18	0.57
1:D:489:LEU:N	1:D:489:LEU:HD23	2.19	0.57
1:E:247:GLN:N	1:E:248:PRO:HD2	2.20	0.57
1:E:312:MET:C	1:E:313:ILE:HD12	2.25	0.57
1:D:269:PRO:HG2	1:D:301:MET:CE	2.34	0.57
1:A:291:VAL:HG11	1:A:421:SER:CB	2.35	0.57
1:A:239:LYS:HB3	1:A:239:LYS:NZ	2.20	0.57
1:E:273:PRO:HB3	1:E:456:ILE:HG22	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:ASP:HB3	1:E:316:ASP:N	2.18	0.56
1:E:246:THR:HG22	1:E:248:PRO:CD	2.31	0.56
1:D:470:ARG:HB2	1:D:536:PRO:HG3	1.88	0.56
1:G:293:TRP:HB2	1:G:437:MET:HB3	1.87	0.56
1:B:300:TYR:CE2	1:B:314:ASP:HB3	2.40	0.56
1:D:278:LYS:HG3	1:D:557:MET:HE1	1.86	0.56
1:G:461:PRO:HD2	1:G:464:LEU:HD22	1.86	0.56
1:G:510:TYR:HD2	1:G:529:GLN:CD	2.08	0.56
1:F:475:ARG:HG3	1:F:484:GLN:O	2.05	0.56
1:D:313:ILE:HD12	1:D:313:ILE:N	2.20	0.56
1:C:293:TRP:HD1	1:C:424:LEU:HD21	1.69	0.56
1:E:246:THR:CG2	1:E:248:PRO:HD2	2.32	0.56
1:D:236:VAL:CG2	1:D:355:ALA:HB1	2.35	0.56
1:D:506:GLU:O	1:D:509:GLN:HG2	2.06	0.56
1:B:377:PHE:HD1	1:B:380:ARG:HH21	1.54	0.56
1:C:316:ASP:O	1:C:317:ASN:CB	2.53	0.56
1:G:467:VAL:HG11	1:G:469:PHE:CZ	2.40	0.56
1:D:293:TRP:CD1	1:D:424:LEU:HD11	2.41	0.56
1:G:342:LEU:HD23	1:G:364:ILE:HG13	1.88	0.56
1:G:459:TRP:CZ2	1:G:461:PRO:HA	2.40	0.56
1:B:385:GLU:HG2	1:B:412:ASN:ND2	2.20	0.56
1:B:232:PHE:HZ	1:B:312:MET:CE	2.19	0.56
1:F:312:MET:HE3	1:F:346:MET:HE3	1.88	0.56
1:G:253:VAL:HG13	1:G:303:LEU:HD23	1.88	0.56
1:A:402:ASP:OD2	1:A:405:GLN:HG2	2.06	0.55
1:E:492:GLY:O	1:E:539:TYR:N	2.39	0.55
1:C:469:PHE:CB	1:C:489:LEU:HB3	2.35	0.55
1:G:386:ARG:O	1:G:391:PRO:HD3	2.06	0.55
1:C:392:ARG:NH2	1:C:406:GLU:OE2	2.40	0.55
1:C:541:THR:O	1:C:545:VAL:HG23	2.06	0.55
1:B:276:MET:HA	1:B:280:ASN:HD22	1.71	0.55
1:G:276:MET:HA	1:G:280:ASN:HD22	1.71	0.55
1:C:300:TYR:CE2	1:C:314:ASP:HB3	2.41	0.55
1:E:467:VAL:HG23	1:E:545:VAL:HG11	1.87	0.55
1:B:520:GLU:HG3	1:B:525:VAL:CG1	2.36	0.55
1:G:361:ILE:HG22	1:G:384:ILE:HD13	1.89	0.55
1:F:333:LEU:O	1:F:395:LYS:HE3	2.06	0.55
1:G:247:GLN:HB3	1:G:248:PRO:CD	2.36	0.55
1:E:517:CYS:HA	1:E:525:VAL:O	2.06	0.55
1:D:549:ILE:O	1:D:552:PRO:HD3	2.06	0.55
1:A:316:ASP:O	1:A:317:ASN:CB	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:555:LYS:O	1:D:559:PHE:HB2	2.06	0.55
1:E:467:VAL:HG22	1:E:545:VAL:HG21	1.88	0.55
1:D:380:ARG:NH1	1:D:448:TYR:N	2.55	0.55
1:F:300:TYR:CE2	1:F:314:ASP:HB3	2.42	0.55
1:E:519:PHE:HE1	1:G:286:LEU:HD23	1.70	0.55
1:D:329:PHE:HD1	1:D:335:MET:HE2	1.71	0.55
1:F:376:ASP:HB3	1:F:379:VAL:HG23	1.88	0.55
1:G:358:ARG:NH1	1:G:411:ARG:NE	2.53	0.55
1:G:300:TYR:HA	1:G:313:ILE:O	2.07	0.55
1:C:365:ILE:N	1:C:365:ILE:HD12	2.22	0.55
1:E:367:PHE:O	1:E:370:GLN:HB2	2.06	0.55
1:E:522:ASN:CA	1:G:286:LEU:HD21	2.37	0.55
1:A:543:MET:HA	1:A:543:MET:HE3	1.89	0.54
1:B:260:PHE:CG	1:B:366:LYS:HD2	2.42	0.54
1:C:368:ASN:O	1:C:369:SER:HB2	2.07	0.54
1:B:238:VAL:HG21	1:B:407:PRO:O	2.07	0.54
1:B:260:PHE:CD2	1:B:366:LYS:HD2	2.41	0.54
1:G:229:GLY:HA2	1:G:243:GLN:HE22	1.71	0.54
1:D:356:VAL:O	1:D:356:VAL:HG12	2.05	0.54
1:B:347:ILE:HD13	1:B:360:LEU:CD2	2.37	0.54
1:G:518:LYS:HE2	1:G:527:MET:HG3	1.90	0.54
1:E:235:GLY:O	1:E:236:VAL:HG23	2.07	0.54
1:E:380:ARG:HH12	1:E:448:TYR:N	2.05	0.54
1:D:329:PHE:CD1	1:D:335:MET:HE2	2.43	0.54
1:B:232:PHE:HZ	1:B:312:MET:HE2	1.71	0.54
1:B:280:ASN:O	1:B:283:LEU:HD12	2.08	0.54
1:F:474:THR:HG22	1:F:476:MET:HG2	1.89	0.54
1:G:487:GLY:H	1:G:503:VAL:CG2	2.20	0.54
1:B:418:ILE:HA	1:B:421:SER:OG	2.08	0.54
1:F:358:ARG:HD3	1:F:411:ARG:HD2	1.90	0.54
1:G:504:THR:HG22	1:G:505:LYS:N	2.15	0.54
1:C:315:ARG:NE	1:C:533:LYS:HZ1	2.02	0.54
1:E:424:LEU:O	1:E:425:LEU:HG	2.07	0.54
1:C:517:CYS:HB3	1:C:525:VAL:O	2.08	0.54
1:B:389:ILE:HD11	1:B:411:ARG:HA	1.90	0.54
1:A:327:PHE:HD1	1:A:392:ARG:HD2	1.71	0.54
1:D:505:LYS:HG3	1:D:506:GLU:N	2.23	0.54
1:D:539:TYR:CE2	1:D:543:MET:HG2	2.43	0.54
1:E:375:CYS:HB3	1:E:379:VAL:HG11	1.90	0.54
1:E:476:MET:O	1:E:483:PRO:HB3	2.08	0.54
1:A:475:ARG:HA	1:A:485:ASN:HB3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:ILE:HD12	1:F:313:ILE:N	2.22	0.53
1:E:389:ILE:HG22	1:E:390:SER:N	2.21	0.53
1:G:488:LEU:HD22	1:G:500:GLN:HG2	1.89	0.53
1:A:233:LEU:CG	1:A:236:VAL:CG2	2.81	0.53
1:F:496:ARG:HB2	1:F:497:PRO:CD	2.28	0.53
1:A:276:MET:HE2	1:A:457:LEU:HD12	1.90	0.53
1:A:363:ASP:OD1	1:A:448:TYR:HD1	1.92	0.53
1:F:277:ASP:H	1:F:280:ASN:HB2	1.72	0.53
1:E:360:LEU:HA	1:E:411:ARG:O	2.08	0.53
1:G:247:GLN:HB3	1:G:248:PRO:HD3	1.90	0.53
1:C:435:HIS:CD2	1:C:436:GLU:H	2.27	0.53
1:E:494:TYR:HD2	1:E:496:ARG:O	1.91	0.53
1:E:307:THR:HG23	1:E:336:HIS:CE1	2.43	0.53
1:C:278:LYS:HE2	1:C:551:ASN:HD21	1.74	0.53
1:F:358:ARG:HG2	1:F:409:SER:HB3	1.90	0.53
1:B:518:LYS:O	1:B:525:VAL:HG12	2.07	0.53
1:B:530:ARG:HG2	1:B:533:LYS:HD2	1.89	0.53
1:F:291:VAL:HG13	1:F:416:PHE:CD1	2.43	0.53
1:E:469:PHE:CG	1:E:489:LEU:HB3	2.43	0.53
1:F:469:PHE:CD2	1:F:489:LEU:HD13	2.44	0.53
1:D:293:TRP:CE3	1:D:293:TRP:O	2.61	0.53
1:D:329:PHE:CD1	1:D:335:MET:CE	2.92	0.53
1:G:367:PHE:CE1	1:G:387:GLU:HB3	2.44	0.53
1:C:489:LEU:C	1:C:490:TYR:CD2	2.82	0.53
1:F:538:ALA:HB3	1:F:541:THR:OG1	2.09	0.53
1:A:246:THR:HG22	1:A:248:PRO:HG2	1.91	0.53
1:D:424:LEU:HD21	1:D:440:LEU:HD21	1.90	0.53
1:E:300:TYR:HA	1:E:313:ILE:O	2.08	0.53
1:A:348:ILE:HG22	1:A:348:ILE:O	2.08	0.53
1:F:291:VAL:HG13	1:F:416:PHE:CE1	2.44	0.53
1:C:376:ASP:OD2	1:C:445:THR:CG2	2.56	0.53
1:F:358:ARG:HG3	1:F:409:SER:HB3	1.90	0.53
1:F:468:ASP:O	1:F:537:ASN:ND2	2.42	0.53
1:E:566:THR:HG22	1:E:566:THR:O	2.08	0.53
1:D:418:ILE:O	1:D:421:SER:OG	2.26	0.53
1:B:470:ARG:HD3	1:B:514:ILE:HD11	1.91	0.53
1:D:293:TRP:HA	1:D:440:LEU:HD23	1.89	0.52
1:C:264:GLU:OE1	1:F:282:LYS:HE2	2.09	0.52
1:D:347:ILE:HG13	1:D:347:ILE:O	2.08	0.52
1:B:273:PRO:CG	1:B:458:LYS:HE3	2.38	0.52
1:F:418:ILE:O	1:F:421:SER:OG	2.26	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ILE:CG2	1:A:530:ARG:HB3	2.40	0.52
1:E:538:ALA:HB3	1:E:541:THR:OG1	2.10	0.52
1:D:329:PHE:C	1:D:329:PHE:HD2	2.13	0.52
1:D:327:PHE:CD1	1:D:392:ARG:HD2	2.45	0.52
1:B:367:PHE:CE1	1:B:387:GLU:HB3	2.44	0.52
1:C:380:ARG:NH1	1:C:448:TYR:N	2.57	0.52
1:D:469:PHE:HB3	1:D:489:LEU:HB3	1.91	0.52
1:D:539:TYR:C	1:D:539:TYR:CD2	2.82	0.52
1:A:460:LYS:HG3	1:A:461:PRO:HD2	1.92	0.52
1:E:233:LEU:HD21	1:E:348:ILE:CD1	2.35	0.52
1:C:294:LYS:HZ3	1:C:460:LYS:HZ2	1.58	0.52
1:A:302:MET:HE3	1:A:359:TYR:CE2	2.45	0.52
1:C:363:ASP:OD1	1:C:448:TYR:HD1	1.92	0.52
1:G:510:TYR:HB3	1:G:529:GLN:NE2	2.25	0.52
1:A:333:LEU:HD22	1:A:395:LYS:HD2	1.91	0.52
1:C:358:ARG:HD3	1:C:411:ARG:HD2	1.91	0.52
1:E:494:TYR:HB2	1:E:539:TYR:HD1	1.73	0.52
1:C:539:TYR:O	1:C:542:ALA:HB3	2.09	0.52
1:G:526:PHE:HD2	1:G:526:PHE:C	2.13	0.52
1:G:312:MET:HE2	1:G:346:MET:CE	2.40	0.52
1:C:329:PHE:CE2	1:C:331:LYS:HB2	2.45	0.52
1:C:496:ARG:HB3	1:C:497:PRO:HD2	1.92	0.52
1:D:233:LEU:HD12	1:D:346:MET:HB3	1.92	0.52
1:B:395:LYS:HB3	1:B:401:ILE:HG13	1.92	0.52
1:F:346:MET:HE2	1:F:359:TYR:CD1	2.42	0.52
1:B:418:ILE:O	1:B:421:SER:OG	2.28	0.52
1:B:363:ASP:OD1	1:B:448:TYR:HD1	1.92	0.52
1:F:546:CYS:O	1:F:549:ILE:HG12	2.09	0.52
1:E:388:ILE:HG22	1:E:388:ILE:O	2.09	0.52
1:F:312:MET:HE3	1:F:346:MET:HE1	1.92	0.52
1:B:520:GLU:O	1:B:521:ASN:C	2.47	0.52
1:B:422:ARG:HB3	1:B:562:ILE:CG2	2.40	0.52
1:G:354:GLN:HG3	1:G:355:ALA:H	1.75	0.52
1:G:403:LYS:NZ	1:G:411:ARG:HH22	2.06	0.51
1:E:356:VAL:CG1	1:E:358:ARG:HH21	2.23	0.51
1:C:499:ALA:HB1	1:C:524:TRP:CD1	2.45	0.51
1:C:294:LYS:NZ	1:C:460:LYS:NZ	2.58	0.51
1:G:232:PHE:CG	1:G:241:VAL:HG11	2.46	0.51
1:B:236:VAL:HG11	1:B:348:ILE:HD11	1.93	0.51
1:F:510:TYR:O	1:F:513:LYS:HB2	2.09	0.51
1:C:342:LEU:HD13	1:C:361:ILE:HD13	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:HD3	1:B:411:ARG:NE	2.26	0.51
1:G:386:ARG:HB2	1:G:386:ARG:HH11	1.76	0.51
1:F:245:THR:HG22	1:F:245:THR:O	2.11	0.51
1:F:543:MET:HE3	1:F:543:MET:HA	1.92	0.51
1:C:467:VAL:CG2	1:C:545:VAL:HG11	2.40	0.51
1:E:268:PHE:CE1	1:E:301:MET:HG3	2.46	0.51
1:C:293:TRP:HB3	1:C:437:MET:SD	2.50	0.51
1:B:396:MET:HG2	1:B:401:ILE:HG21	1.92	0.51
1:F:469:PHE:CB	1:F:489:LEU:HB3	2.41	0.51
1:C:387:GLU:OE1	1:C:387:GLU:HA	2.10	0.51
1:B:396:MET:SD	1:B:403:LYS:HD3	2.51	0.51
1:D:251:GLY:O	1:D:255:GLN:HB2	2.11	0.51
1:F:350:ARG:HA	1:F:354:GLN:O	2.11	0.51
1:D:529:GLN:HG2	1:D:530:ARG:N	2.25	0.51
1:G:545:VAL:O	1:G:549:ILE:HG23	2.10	0.51
1:B:535:PHE:CD1	1:B:536:PRO:HD2	2.46	0.51
1:G:462:PRO:HD2	1:G:555:LYS:NZ	2.25	0.51
1:A:519:PHE:HE1	1:E:286:LEU:HD23	1.75	0.51
1:E:268:PHE:CZ	1:E:301:MET:HG3	2.46	0.51
1:D:232:PHE:HB2	1:D:320:PHE:CD2	2.46	0.51
1:B:385:GLU:HG2	1:B:412:ASN:HD21	1.76	0.51
1:B:471:LEU:HD12	1:B:472:LYS:N	2.26	0.51
1:E:230:ALA:HA	1:E:243:GLN:OE1	2.11	0.51
1:B:356:VAL:O	1:B:356:VAL:HG12	2.09	0.51
1:G:246:THR:CG2	1:G:248:PRO:HD2	2.40	0.51
1:D:477:GLY:HA2	1:D:483:PRO:CB	2.41	0.51
1:B:368:ASN:O	1:B:369:SER:HB2	2.09	0.51
1:E:239:LYS:O	1:E:407:PRO:HB3	2.10	0.51
1:E:542:ALA:O	1:E:545:VAL:HB	2.11	0.50
1:B:288:PRO:HD3	1:C:498:PHE:CE2	2.46	0.50
1:B:357:PRO:HB2	1:B:408:PHE:HB3	1.91	0.50
1:D:329:PHE:C	1:D:329:PHE:CD2	2.85	0.50
1:D:390:SER:O	1:D:394:GLU:HG2	2.11	0.50
1:C:245:THR:HG22	1:C:245:THR:O	2.11	0.50
1:A:287:LYS:HB2	1:A:288:PRO:CD	2.41	0.50
1:C:461:PRO:HD2	1:C:464:LEU:HD13	1.93	0.50
1:B:402:ASP:HB3	1:B:405:GLN:HG2	1.94	0.50
1:C:467:VAL:HB	1:C:469:PHE:CE2	2.47	0.50
1:F:244:VAL:O	1:F:250:LEU:HD13	2.11	0.50
1:A:471:LEU:HD12	1:A:471:LEU:C	2.31	0.50
1:C:325:LEU:HD11	1:C:408:PHE:HE1	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:THR:HG22	1:B:400:LEU:H	1.76	0.50
1:A:313:ILE:N	1:A:313:ILE:HD12	2.27	0.50
1:G:346:MET:HE1	1:G:359:TYR:CB	2.40	0.50
1:C:283:LEU:HA	1:C:286:LEU:HG	1.92	0.50
1:C:315:ARG:HE	1:C:533:LYS:HZ3	1.58	0.50
1:F:539:TYR:C	1:F:539:TYR:CD2	2.84	0.50
1:F:282:LYS:O	1:F:286:LEU:HD13	2.11	0.50
1:F:438:ASP:O	1:F:460:LYS:HG3	2.11	0.50
1:F:422:ARG:HD3	1:F:563:ASP:OD1	2.11	0.50
1:A:539:TYR:CE2	1:A:543:MET:HG3	2.45	0.50
1:D:467:VAL:HG11	1:D:469:PHE:CE1	2.46	0.50
1:A:435:HIS:CG	1:A:436:GLU:H	2.29	0.50
1:B:380:ARG:HH12	1:B:448:TYR:N	2.09	0.50
1:E:481:LEU:O	1:E:483:PRO:HD3	2.12	0.50
1:G:488:LEU:CD2	1:G:500:GLN:HG2	2.42	0.50
1:B:246:THR:HG22	1:B:248:PRO:CD	2.16	0.50
1:E:293:TRP:CE3	1:E:293:TRP:O	2.65	0.50
1:E:419:CYS:HB3	1:E:566:THR:HG23	1.91	0.50
1:C:469:PHE:HB3	1:C:489:LEU:HB3	1.92	0.50
1:D:396:MET:HG2	1:D:401:ILE:HB	1.93	0.50
1:D:554:THR:H	1:D:557:MET:HB3	1.77	0.50
1:F:312:MET:HE1	1:F:346:MET:HE1	1.93	0.50
1:C:503:VAL:CG1	1:C:508:LYS:HE3	2.41	0.50
1:G:330:ARG:NH1	1:G:386:ARG:NH2	2.60	0.50
1:D:422:ARG:HD3	1:D:563:ASP:OD1	2.11	0.50
1:E:533:LYS:HG2	1:E:535:PHE:O	2.11	0.50
1:C:294:LYS:HZ2	1:C:458:LYS:CE	2.22	0.50
1:E:396:MET:HG2	1:E:401:ILE:HB	1.94	0.50
1:E:468:ASP:HB2	1:E:537:ASN:OD1	2.12	0.50
1:G:375:CYS:HB3	1:G:379:VAL:HG11	1.93	0.50
1:A:380:ARG:NH1	1:A:448:TYR:N	2.60	0.50
1:A:511:ASP:C	1:A:513:LYS:H	2.16	0.50
1:D:367:PHE:CE1	1:D:387:GLU:HB3	2.47	0.50
1:D:516:GLU:HG2	1:D:527:MET:HG3	1.93	0.50
1:B:376:ASP:HB3	1:B:379:VAL:HG23	1.93	0.50
1:F:275:SER:O	1:F:280:ASN:ND2	2.44	0.49
1:B:486:VAL:HG23	1:B:486:VAL:O	2.12	0.49
1:F:247:GLN:N	1:F:248:PRO:HD2	2.27	0.49
1:E:236:VAL:HG12	1:E:237:THR:N	2.28	0.49
1:C:260:PHE:CG	1:C:366:LYS:HD2	2.47	0.49
1:F:300:TYR:HA	1:F:313:ILE:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:ARG:HD3	1:E:411:ARG:HD3	1.92	0.49
1:E:325:LEU:HA	1:E:406:GLU:HG2	1.94	0.49
1:C:248:PRO:O	1:C:252:GLU:HB2	2.11	0.49
1:E:232:PHE:CD1	1:E:238:VAL:HG21	2.47	0.49
1:B:543:MET:CE	1:B:543:MET:HA	2.42	0.49
1:E:358:ARG:HG3	1:E:409:SER:HB3	1.94	0.49
1:D:513:LYS:HB3	1:D:529:GLN:HE21	1.78	0.49
1:G:358:ARG:HH11	1:G:411:ARG:NE	2.03	0.49
1:A:530:ARG:HG2	1:A:530:ARG:NH1	2.27	0.49
1:B:240:GLY:HA3	1:B:323:SER:HB2	1.95	0.49
1:C:425:LEU:HD13	1:C:559:PHE:CD1	2.47	0.49
1:G:418:ILE:O	1:G:418:ILE:HG22	2.11	0.49
1:A:529:GLN:HG2	1:A:530:ARG:N	2.27	0.49
1:A:401:ILE:O	1:A:401:ILE:HG22	2.13	0.49
1:E:233:LEU:HD23	1:E:233:LEU:C	2.33	0.49
1:D:467:VAL:CG1	1:D:469:PHE:CE1	2.96	0.49
1:A:293:TRP:CB	1:A:437:MET:SD	3.01	0.49
1:E:232:PHE:HB2	1:E:320:PHE:CE2	2.47	0.49
1:D:488:LEU:HB2	1:D:490:TYR:HE2	1.77	0.49
1:F:236:VAL:HG23	1:F:348:ILE:HD13	1.94	0.49
1:B:372:VAL:O	1:B:375:CYS:HB2	2.13	0.49
1:B:535:PHE:HD1	1:B:536:PRO:HD2	1.78	0.49
1:C:291:VAL:HG11	1:C:421:SER:HB2	1.95	0.49
1:F:417:ASP:CG	1:F:418:ILE:H	2.16	0.48
1:D:467:VAL:HG23	1:D:545:VAL:HG11	1.95	0.48
1:F:358:ARG:HG3	1:F:409:SER:CB	2.43	0.48
1:A:307:THR:HG23	1:A:336:HIS:ND1	2.28	0.48
1:G:526:PHE:HD2	1:G:526:PHE:O	1.95	0.48
1:A:293:TRP:HA	1:A:440:LEU:HD23	1.95	0.48
1:D:268:PHE:HE1	1:D:301:MET:HG3	1.78	0.48
1:F:231:ILE:HG21	1:F:234:GLU:HG3	1.95	0.48
1:B:358:ARG:HH11	1:B:411:ARG:NH2	2.10	0.48
1:G:249:LYS:HD2	1:G:252:GLU:OE1	2.13	0.48
1:B:329:PHE:HD2	1:B:330:ARG:N	2.11	0.48
1:G:546:CYS:HA	1:G:549:ILE:HD13	1.95	0.48
1:A:326:GLU:OE1	1:A:401:ILE:HD11	2.13	0.48
1:E:235:GLY:O	1:E:236:VAL:CG2	2.62	0.48
1:G:327:PHE:CD1	1:G:392:ARG:HD2	2.48	0.48
1:E:473:ILE:HD11	1:E:485:ASN:OD1	2.13	0.48
1:A:398:THR:HG22	1:A:398:THR:O	2.13	0.48
1:A:247:GLN:N	1:A:248:PRO:CD	2.75	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:THR:HG22	1:D:507:LEU:HD13	1.94	0.48
1:B:291:VAL:CG2	1:B:292:SER:N	2.76	0.48
1:E:377:PHE:O	1:E:381:LEU:HB2	2.14	0.48
1:F:469:PHE:CG	1:F:489:LEU:HB3	2.49	0.48
1:F:230:ALA:CB	1:F:243:GLN:CD	2.82	0.48
1:C:232:PHE:CD1	1:C:241:VAL:HG11	2.48	0.48
1:F:255:GLN:O	1:F:259:GLN:HG3	2.14	0.48
1:B:542:ALA:O	1:B:545:VAL:HB	2.14	0.48
1:E:519:PHE:CE1	1:G:286:LEU:HD23	2.47	0.48
1:C:473:ILE:HD13	1:C:503:VAL:HG11	1.95	0.48
1:E:461:PRO:HG2	1:E:464:LEU:HG	1.96	0.48
1:E:347:ILE:O	1:E:347:ILE:HG13	2.12	0.48
1:A:273:PRO:HB2	1:A:458:LYS:HD3	1.95	0.48
1:C:511:ASP:O	1:C:512:ASN:HB2	2.13	0.48
1:B:247:GLN:N	1:B:248:PRO:CD	2.77	0.48
1:F:468:ASP:H	1:F:537:ASN:HD21	1.60	0.48
1:B:376:ASP:O	1:B:379:VAL:HB	2.14	0.48
1:F:467:VAL:HG22	1:F:469:PHE:CZ	2.49	0.47
1:B:380:ARG:NH1	1:B:448:TYR:N	2.62	0.47
1:E:422:ARG:HH21	1:E:423:LYS:NZ	2.12	0.47
1:B:232:PHE:CZ	1:B:312:MET:HE2	2.49	0.47
1:A:418:ILE:HG22	1:A:562:ILE:HG13	1.95	0.47
1:E:287:LYS:HB2	1:E:288:PRO:CD	2.45	0.47
1:D:518:LYS:HB3	1:D:518:LYS:HE3	1.51	0.47
1:F:537:ASN:HD22	1:F:537:ASN:H	0.71	0.47
1:B:287:LYS:HB2	1:B:288:PRO:CD	2.44	0.47
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.68	0.47
1:A:422:ARG:CG	1:A:423:LYS:N	2.77	0.47
1:G:482:LEU:HA	1:G:483:PRO:HD2	1.82	0.47
1:C:367:PHE:CE1	1:C:387:GLU:HB3	2.49	0.47
1:D:286:LEU:HD23	1:D:286:LEU:N	2.29	0.47
1:E:472:LYS:NZ	1:E:474:THR:HG21	2.29	0.47
1:F:489:LEU:HD21	1:F:501:ILE:CG2	2.40	0.47
1:D:519:PHE:CZ	1:D:522:ASN:HA	2.50	0.47
1:F:232:PHE:HB2	1:F:320:PHE:CE2	2.50	0.47
1:D:271:ALA:HB2	1:D:449:LYS:O	2.15	0.47
1:A:543:MET:CA	1:A:543:MET:HE3	2.44	0.47
1:D:278:LYS:HD3	1:D:557:MET:HE3	1.95	0.47
1:B:260:PHE:HA	1:B:366:LYS:HE3	1.97	0.47
1:G:473:ILE:HD13	1:G:503:VAL:CG1	2.45	0.47
1:G:363:ASP:OD1	1:G:448:TYR:HD1	1.98	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:NZ	1:B:239:LYS:HB2	2.30	0.47
1:E:424:LEU:O	1:E:425:LEU:CB	2.62	0.47
1:F:529:GLN:HG3	1:F:530:ARG:N	2.30	0.47
1:D:471:LEU:CD2	1:D:507:LEU:HD23	2.44	0.47
1:D:422:ARG:HA	1:D:559:PHE:HE2	1.79	0.47
1:D:422:ARG:HG3	1:D:559:PHE:CE2	2.50	0.47
1:E:494:TYR:CD1	1:E:539:TYR:CD1	3.03	0.47
1:G:513:LYS:HB3	1:G:529:GLN:HE21	1.79	0.47
1:A:425:LEU:CD2	1:A:555:LYS:HE3	2.44	0.47
1:F:347:ILE:HD12	1:F:349:ASP:HB2	1.96	0.47
1:C:467:VAL:HG23	1:C:545:VAL:HG11	1.97	0.47
1:E:546:CYS:HA	1:E:549:ILE:HD12	1.97	0.47
1:B:291:VAL:HG22	1:B:292:SER:N	2.30	0.47
1:C:389:ILE:HG22	1:C:390:SER:N	2.30	0.47
1:A:233:LEU:CB	1:A:236:VAL:HG23	2.37	0.47
1:E:420:THR:O	1:E:420:THR:CG2	2.61	0.47
1:B:358:ARG:HH12	1:B:411:ARG:HH21	1.60	0.47
1:C:491:VAL:HG11	1:C:542:ALA:HB2	1.97	0.47
1:D:470:ARG:NH2	1:D:536:PRO:HD3	2.30	0.47
1:B:236:VAL:HG12	1:B:348:ILE:HD11	1.93	0.46
1:F:527:MET:HG3	1:F:528:ARG:N	2.30	0.46
1:E:358:ARG:HH11	1:E:411:ARG:NH1	2.12	0.46
1:E:381:LEU:HD12	1:E:381:LEU:HA	1.72	0.46
1:A:526:PHE:C	1:A:526:PHE:CD2	2.88	0.46
1:A:322:VAL:HG12	1:A:407:PRO:HG2	1.96	0.46
1:B:232:PHE:CZ	1:B:312:MET:CE	2.98	0.46
1:C:329:PHE:HD2	1:C:331:LYS:N	2.07	0.46
1:E:309:GLU:OE1	1:E:309:GLU:CA	2.59	0.46
1:D:358:ARG:HD3	1:D:411:ARG:CD	2.44	0.46
1:E:278:LYS:HD2	1:E:551:ASN:OD1	2.14	0.46
1:C:491:VAL:CG2	1:C:539:TYR:HA	2.43	0.46
1:F:363:ASP:OD1	1:F:448:TYR:CD1	2.68	0.46
1:G:467:VAL:CG1	1:G:469:PHE:CZ	2.98	0.46
1:F:437:MET:O	1:F:437:MET:HG3	2.15	0.46
1:B:468:ASP:N	1:B:468:ASP:OD1	2.48	0.46
1:B:232:PHE:CE1	1:B:241:VAL:HG11	2.50	0.46
1:F:560:GLU:HA	1:F:563:ASP:OD2	2.16	0.46
1:E:521:ASN:O	1:E:522:ASN:HB2	2.15	0.46
1:C:236:VAL:HB	1:C:348:ILE:HD11	1.97	0.46
1:D:234:GLU:OE2	1:D:234:GLU:HA	2.14	0.46
1:D:438:ASP:O	1:D:460:LYS:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:ILE:HD11	1:D:561:PHE:CB	2.45	0.46
1:E:278:LYS:HG2	1:E:557:MET:CE	2.46	0.46
1:F:312:MET:C	1:F:313:ILE:HD12	2.36	0.46
1:C:471:LEU:O	1:C:472:LYS:HG3	2.15	0.46
1:G:378:ASN:ND2	1:G:378:ASN:H	2.13	0.46
1:C:462:PRO:CD	1:C:555:LYS:HE3	2.28	0.46
1:A:246:THR:HG22	1:A:248:PRO:CD	2.44	0.46
1:F:293:TRP:CD1	1:F:293:TRP:N	2.83	0.46
1:D:248:PRO:O	1:D:252:GLU:HB2	2.16	0.46
1:D:511:ASP:OD1	1:D:512:ASN:ND2	2.48	0.46
1:C:469:PHE:CG	1:C:489:LEU:HB3	2.50	0.46
1:D:539:TYR:CE2	1:D:543:MET:CG	2.99	0.46
1:G:400:LEU:HD12	1:G:400:LEU:H	1.81	0.46
1:A:294:LYS:HE2	2:A:5:SO4:O4	2.15	0.46
1:C:328:PRO:HD2	1:C:392:ARG:HG2	1.97	0.46
1:B:250:LEU:HD23	1:B:251:GLY:N	2.31	0.46
1:E:556:GLU:H	1:E:556:GLU:CD	2.18	0.46
1:G:346:MET:HE1	1:G:359:TYR:CG	2.51	0.46
1:A:519:PHE:CG	1:A:549:ILE:HD12	2.51	0.46
1:F:302:MET:HE2	1:F:312:MET:SD	2.56	0.46
1:B:286:LEU:CD1	1:C:519:PHE:HE1	2.28	0.46
1:G:520:GLU:O	1:G:521:ASN:C	2.54	0.46
1:G:511:ASP:C	1:G:513:LYS:N	2.68	0.46
1:G:494:TYR:CD2	1:G:539:TYR:CE1	3.04	0.46
1:C:471:LEU:HD22	1:C:515:ILE:HD13	1.97	0.46
1:C:405:GLN:OE1	1:C:405:GLN:HA	2.15	0.46
1:B:236:VAL:HG13	1:B:237:THR:N	2.30	0.46
1:F:533:LYS:HD2	1:F:533:LYS:HA	1.81	0.46
1:A:246:THR:HG22	1:A:248:PRO:CG	2.46	0.46
1:B:347:ILE:HG13	1:B:347:ILE:O	2.15	0.46
1:A:449:LYS:HG2	1:A:450:PRO:HD2	1.98	0.46
1:B:330:ARG:HB2	1:B:391:PRO:HG3	1.96	0.46
1:F:367:PHE:O	1:F:370:GLN:HB2	2.16	0.46
1:B:381:LEU:HA	1:B:381:LEU:HD23	1.72	0.46
1:B:386:ARG:HB2	1:B:386:ARG:NH1	2.31	0.46
1:D:519:PHE:CD2	1:D:549:ILE:HD12	2.51	0.46
1:C:498:PHE:C	1:C:498:PHE:HD2	2.18	0.46
1:F:517:CYS:HB3	1:F:525:VAL:O	2.15	0.46
1:G:494:TYR:CE1	1:G:496:ARG:HG2	2.51	0.46
1:G:293:TRP:HE3	1:G:293:TRP:O	1.99	0.46
1:D:312:MET:C	1:D:313:ILE:HD12	2.36	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:GLN:N	1:B:248:PRO:HD3	2.31	0.45
1:E:278:LYS:HB2	1:E:551:ASN:HD21	1.81	0.45
1:E:522:ASN:HA	1:G:286:LEU:CD2	2.46	0.45
1:G:510:TYR:HD2	1:G:529:GLN:OE1	2.00	0.45
1:G:397:LYS:O	1:F:414:PRO:HB2	2.16	0.45
1:A:328:PRO:HD2	1:A:392:ARG:HG2	1.99	0.45
1:E:363:ASP:OD1	1:E:448:TYR:CD1	2.68	0.45
1:D:329:PHE:CD2	1:D:330:ARG:N	2.83	0.45
1:G:479:GLU:CD	1:G:479:GLU:H	2.19	0.45
1:E:316:ASP:O	1:E:317:ASN:CB	2.61	0.45
1:F:233:LEU:HD21	1:F:348:ILE:HG13	1.97	0.45
1:E:477:GLY:HA2	1:E:483:PRO:HB3	1.99	0.45
1:A:527:MET:HG3	1:A:528:ARG:HG3	1.98	0.45
1:B:276:MET:HE2	1:B:281:ILE:HA	1.99	0.45
1:D:269:PRO:HG2	1:D:301:MET:HE1	1.96	0.45
1:C:406:GLU:HB2	1:C:407:PRO:HD2	1.99	0.45
1:B:322:VAL:HG12	1:B:407:PRO:HG2	1.99	0.45
1:C:307:THR:HG23	1:C:308:ASN:H	1.81	0.45
1:G:255:GLN:O	1:G:259:GLN:HG3	2.17	0.45
1:E:491:VAL:HG11	1:E:498:PHE:HD1	1.81	0.45
1:E:244:VAL:O	1:E:244:VAL:HG12	2.16	0.45
1:A:327:PHE:CE1	1:A:392:ARG:HD2	2.49	0.45
1:F:244:VAL:HG23	1:F:250:LEU:HB2	1.99	0.45
1:G:528:ARG:HG3	1:G:529:GLN:N	2.32	0.45
1:D:398:THR:HG21	1:D:400:LEU:HD22	1.98	0.45
1:G:312:MET:HE2	1:G:346:MET:HE3	1.98	0.45
1:E:550:SER:O	1:E:552:PRO:HD3	2.16	0.45
1:C:287:LYS:HB2	1:C:288:PRO:CD	2.47	0.45
1:F:561:PHE:C	1:F:561:PHE:CD2	2.89	0.45
1:C:294:LYS:HZ3	1:C:460:LYS:NZ	2.15	0.45
1:B:300:TYR:HA	1:B:313:ILE:O	2.16	0.45
1:D:244:VAL:O	1:D:244:VAL:CG2	2.64	0.45
1:C:386:ARG:O	1:C:391:PRO:HD3	2.16	0.45
1:E:293:TRP:HE3	1:E:293:TRP:O	1.98	0.45
1:E:314:ASP:HB2	1:E:318:SER:HB2	1.99	0.45
1:B:543:MET:HE3	1:B:543:MET:HA	1.98	0.45
1:C:498:PHE:C	1:C:498:PHE:CD2	2.89	0.45
1:G:243:GLN:HB2	1:G:320:PHE:CE2	2.51	0.45
1:F:357:PRO:HB2	1:F:408:PHE:HB3	1.98	0.45
1:C:527:MET:HG3	1:C:528:ARG:H	1.82	0.45
1:A:233:LEU:HD12	1:A:234:GLU:N	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:346:MET:CE	1:G:359:TYR:HB2	2.46	0.45
1:D:513:LYS:HG2	1:D:529:GLN:NE2	2.31	0.45
1:F:307:THR:HG23	1:F:308:ASN:N	2.32	0.45
1:D:549:ILE:HG13	1:D:550:SER:N	2.32	0.45
1:B:348:ILE:HD12	1:B:355:ALA:HB1	1.99	0.45
1:A:460:LYS:HG3	1:A:461:PRO:CD	2.47	0.45
1:E:487:GLY:C	1:E:488:LEU:HD23	2.37	0.45
1:B:487:GLY:O	1:B:500:GLN:HA	2.17	0.45
1:A:375:CYS:HB3	1:A:379:VAL:HG11	1.98	0.45
1:C:489:LEU:C	1:C:490:TYR:HD2	2.20	0.44
1:G:312:MET:CE	1:G:346:MET:HE2	2.47	0.44
1:E:395:LYS:HB3	1:E:401:ILE:CG1	2.46	0.44
1:A:367:PHE:CZ	1:A:387:GLU:HB3	2.52	0.44
1:D:329:PHE:HD2	1:D:331:LYS:H	1.65	0.44
1:C:278:LYS:HG3	1:C:551:ASN:HD21	1.82	0.44
1:B:370:GLN:HA	1:B:371:PRO:HD3	1.60	0.44
1:F:422:ARG:HG3	1:F:562:ILE:CG2	2.47	0.44
1:C:294:LYS:HZ1	1:C:460:LYS:HZ1	1.64	0.44
1:E:329:PHE:HD2	1:E:331:LYS:H	1.63	0.44
1:G:469:PHE:CB	1:G:489:LEU:HB3	2.47	0.44
1:E:368:ASN:O	1:E:369:SER:HB2	2.17	0.44
1:B:471:LEU:HD23	1:B:515:ILE:HD13	1.99	0.44
1:E:230:ALA:CA	1:E:243:GLN:OE1	2.65	0.44
1:G:273:PRO:HB3	1:G:456:ILE:HG22	1.96	0.44
1:D:543:MET:HE3	1:D:543:MET:HA	1.99	0.44
1:G:329:PHE:HD2	1:G:330:ARG:N	2.16	0.44
1:G:311:PHE:HA	1:G:320:PHE:O	2.17	0.44
1:D:376:ASP:OD2	1:D:445:THR:CG2	2.65	0.44
1:E:347:ILE:CD1	1:E:360:LEU:HD11	2.47	0.44
1:E:244:VAL:HG12	1:E:250:LEU:HB2	1.99	0.44
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.66	0.44
1:E:365:ILE:HD12	1:E:365:ILE:N	2.32	0.44
1:A:311:PHE:HA	1:A:320:PHE:O	2.18	0.44
1:E:380:ARG:O	1:E:384:ILE:HG13	2.18	0.44
1:D:424:LEU:CD2	1:D:440:LEU:HD21	2.48	0.44
1:F:494:TYR:CD2	1:F:539:TYR:CD1	3.05	0.44
1:D:233:LEU:O	1:D:233:LEU:HD23	2.17	0.44
1:D:498:PHE:CE1	1:D:542:ALA:HB1	2.53	0.44
1:E:516:GLU:HG2	1:E:527:MET:HG3	1.99	0.44
1:C:470:ARG:HD3	1:C:514:ILE:CD1	2.47	0.44
1:F:519:PHE:CD2	1:F:519:PHE:C	2.90	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:GLN:N	1:C:248:PRO:CD	2.81	0.44
1:A:461:PRO:HA	1:A:462:PRO:HD3	1.84	0.44
1:G:290:LYS:HD3	1:G:417:ASP:HA	2.00	0.44
1:A:329:PHE:HD2	1:A:331:LYS:H	1.66	0.44
1:G:473:ILE:HD13	1:G:503:VAL:HG13	2.00	0.44
1:C:367:PHE:CZ	1:C:387:GLU:HB3	2.52	0.44
1:E:230:ALA:HB2	1:E:243:GLN:OE1	2.17	0.44
1:G:449:LYS:HG2	1:G:450:PRO:O	2.18	0.44
1:A:519:PHE:CD2	1:A:519:PHE:C	2.91	0.44
1:D:392:ARG:NH2	1:D:406:GLU:OE1	2.50	0.44
1:G:288:PRO:HB2	1:G:445:THR:OG1	2.18	0.44
1:D:541:THR:O	1:D:545:VAL:HG23	2.17	0.44
1:F:293:TRP:H	1:F:293:TRP:HD1	1.65	0.44
1:C:473:ILE:CD1	1:C:503:VAL:HG11	2.48	0.44
1:C:335:MET:HE2	1:C:335:MET:HA	1.97	0.44
1:C:554:THR:OG1	1:C:557:MET:CB	2.66	0.44
1:B:520:GLU:HG3	1:B:525:VAL:HG11	1.99	0.44
1:C:311:PHE:C	1:C:312:MET:HG2	2.38	0.44
1:A:488:LEU:HD13	1:A:497:PRO:HG3	2.00	0.44
1:F:346:MET:CE	1:F:359:TYR:HD1	2.27	0.44
1:B:289:TYR:HD2	1:B:442:PHE:HB3	1.83	0.44
1:G:333:LEU:O	1:G:395:LYS:HE3	2.17	0.44
1:E:377:PHE:CZ	1:E:443:GLN:HG2	2.53	0.44
1:G:539:TYR:C	1:G:539:TYR:CD2	2.90	0.44
1:F:461:PRO:HA	1:F:462:PRO:HD3	1.83	0.44
1:E:390:SER:N	1:E:391:PRO:CD	2.81	0.44
1:A:342:LEU:CD1	1:A:361:ILE:HD13	2.48	0.43
1:G:489:LEU:HD23	1:G:489:LEU:N	2.33	0.43
1:B:277:ASP:HA	1:B:553:VAL:CG2	2.48	0.43
1:A:378:ASN:O	1:A:382:GLN:HG3	2.17	0.43
1:D:279:GLN:O	1:D:282:LYS:HB2	2.17	0.43
1:F:422:ARG:HG3	1:F:562:ILE:HG21	1.99	0.43
1:E:462:PRO:HD2	1:E:555:LYS:HE2	1.99	0.43
1:E:269:PRO:HG2	1:E:301:MET:CE	2.48	0.43
1:D:543:MET:HA	1:D:543:MET:CE	2.47	0.43
1:E:501:ILE:CD1	1:E:524:TRP:O	2.66	0.43
1:C:327:PHE:CD1	1:C:392:ARG:HD2	2.53	0.43
1:F:452:ARG:NH1	1:F:454:ASP:OD1	2.51	0.43
1:F:550:SER:C	1:F:552:PRO:HD3	2.39	0.43
1:C:303:LEU:HD12	1:C:340:THR:O	2.19	0.43
1:A:389:ILE:HA	1:A:389:ILE:HD12	1.69	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:VAL:O	1:C:375:CYS:HB2	2.18	0.43
1:F:537:ASN:N	1:F:537:ASN:ND2	2.29	0.43
1:F:556:GLU:O	1:F:560:GLU:HG2	2.18	0.43
1:G:459:TRP:CH2	1:G:461:PRO:HG3	2.54	0.43
1:E:380:ARG:NH1	1:E:448:TYR:N	2.66	0.43
1:E:390:SER:O	1:E:394:GLU:HG3	2.18	0.43
1:C:326:GLU:OE2	1:C:336:HIS:CE1	2.71	0.43
1:B:378:ASN:O	1:B:382:GLN:HG3	2.19	0.43
1:F:471:LEU:HD12	1:F:471:LEU:C	2.39	0.43
1:E:306:GLY:C	1:E:309:GLU:HB2	2.39	0.43
1:B:291:VAL:CG1	1:B:421:SER:HB3	2.49	0.43
1:A:294:LYS:CE	2:A:5:SO4:O4	2.67	0.43
1:A:470:ARG:NH2	1:A:535:PHE:HD1	2.16	0.43
1:B:249:LYS:HE3	1:B:311:PHE:CZ	2.53	0.43
1:D:398:THR:O	1:D:398:THR:CG2	2.66	0.43
1:A:363:ASP:OD1	1:A:448:TYR:CD1	2.71	0.43
1:G:405:GLN:OE1	1:G:405:GLN:N	2.51	0.43
1:C:443:GLN:HA	1:C:444:PRO:HD2	1.91	0.43
1:D:503:VAL:CG1	1:D:508:LYS:HG2	2.49	0.43
1:C:236:VAL:HG23	1:C:348:ILE:HD13	2.00	0.43
1:B:377:PHE:CE2	1:B:443:GLN:HG2	2.54	0.43
1:A:395:LYS:HB2	1:A:401:ILE:HD12	2.01	0.43
1:D:402:ASP:OD1	1:D:405:GLN:HG2	2.19	0.43
1:E:402:ASP:HB3	1:E:405:GLN:CG	2.49	0.43
1:A:363:ASP:C	1:A:384:ILE:HD11	2.39	0.43
1:B:288:PRO:HD3	1:C:498:PHE:CD2	2.54	0.43
1:G:487:GLY:H	1:G:503:VAL:HG21	1.82	0.43
1:B:351:VAL:HG22	1:B:352:ASN:OD1	2.18	0.43
1:C:439:GLY:O	1:C:440:LEU:HD23	2.18	0.43
1:C:556:GLU:CD	1:C:556:GLU:H	2.22	0.43
1:A:327:PHE:HB3	1:A:337:LEU:HD12	2.01	0.43
1:A:416:PHE:CE1	1:A:424:LEU:HD11	2.49	0.43
1:B:344:GLY:HA3	1:B:360:LEU:O	2.19	0.43
1:A:449:LYS:HA	1:A:450:PRO:HD3	1.65	0.43
1:A:402:ASP:HB3	1:A:405:GLN:CG	2.49	0.43
1:A:329:PHE:HD2	1:A:330:ARG:N	2.16	0.43
1:C:337:LEU:HA	1:C:337:LEU:HD23	1.69	0.43
1:A:413:LYS:HG2	1:A:414:PRO:HD2	2.01	0.43
1:E:247:GLN:N	1:E:248:PRO:CD	2.82	0.43
1:G:467:VAL:HG12	1:G:469:PHE:CE2	2.54	0.43
1:E:367:PHE:CZ	1:E:387:GLU:HB3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:ASP:OD2	1:E:404:THR:HB	2.19	0.43
1:D:504:THR:HG23	1:D:506:GLU:HG3	2.00	0.42
1:G:518:LYS:O	1:G:525:VAL:HG22	2.19	0.42
1:D:294:LYS:NZ	1:D:460:LYS:NZ	2.67	0.42
1:B:358:ARG:HG3	1:B:409:SER:HB2	1.99	0.42
1:B:273:PRO:HB3	1:B:456:ILE:CG2	2.49	0.42
1:G:312:MET:CE	1:G:346:MET:CE	2.97	0.42
1:D:546:CYS:HA	1:D:549:ILE:HG12	2.01	0.42
1:F:230:ALA:CB	1:F:243:GLN:OE1	2.62	0.42
1:B:494:TYR:CD2	1:B:539:TYR:CD1	3.07	0.42
1:C:294:LYS:NZ	1:C:460:LYS:HZ2	2.16	0.42
1:A:293:TRP:O	1:A:293:TRP:HE3	2.00	0.42
1:B:333:LEU:HB3	1:B:395:LYS:CE	2.49	0.42
1:F:387:GLU:CA	1:F:387:GLU:OE1	2.63	0.42
1:F:474:THR:CG2	1:F:476:MET:HG2	2.48	0.42
1:C:264:GLU:HG3	1:F:282:LYS:NZ	2.33	0.42
1:A:507:LEU:HD11	1:A:526:PHE:HB2	2.02	0.42
1:C:470:ARG:HD3	1:C:514:ILE:HD11	2.01	0.42
1:B:555:LYS:O	1:B:559:PHE:HB2	2.20	0.42
1:D:278:LYS:HG3	1:D:557:MET:CE	2.49	0.42
1:G:283:LEU:HD23	1:G:286:LEU:CD2	2.47	0.42
1:C:294:LYS:NZ	1:C:458:LYS:HE3	2.30	0.42
1:G:470:ARG:NH2	1:G:535:PHE:HD1	2.15	0.42
1:B:301:MET:O	1:B:313:ILE:HD12	2.20	0.42
1:B:470:ARG:NH1	1:B:536:PRO:HD3	2.35	0.42
1:B:511:ASP:C	1:B:513:LYS:H	2.20	0.42
1:G:366:LYS:HD2	1:G:369:SER:O	2.19	0.42
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.71	0.42
1:F:422:ARG:CD	1:F:563:ASP:OD1	2.68	0.42
1:D:494:TYR:CE1	1:D:539:TYR:CE1	3.07	0.42
1:G:275:SER:O	1:G:280:ASN:ND2	2.53	0.42
1:C:286:LEU:CD1	1:F:522:ASN:O	2.67	0.42
1:B:325:LEU:HD11	1:B:408:PHE:CE1	2.53	0.42
1:D:269:PRO:HG2	1:D:301:MET:HE2	2.01	0.42
1:G:367:PHE:CZ	1:G:387:GLU:HB3	2.55	0.42
1:D:231:ILE:HG21	1:D:234:GLU:HB2	2.01	0.42
1:G:337:LEU:HA	1:G:337:LEU:HD23	1.78	0.42
1:C:385:GLU:HG2	1:C:412:ASN:ND2	2.35	0.42
1:C:316:ASP:O	1:C:317:ASN:HB3	2.20	0.42
1:B:342:LEU:HD13	1:B:361:ILE:HD13	2.01	0.42
1:D:564:ARG:HE	1:D:564:ARG:HB2	1.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ARG:NH1	1:B:452:ARG:HG3	2.34	0.42
1:E:474:THR:O	1:E:485:ASN:HB2	2.19	0.42
1:E:494:TYR:HB2	1:E:539:TYR:CD1	2.54	0.42
1:A:384:ILE:O	1:A:388:ILE:HB	2.19	0.42
1:E:518:LYS:HG2	1:E:519:PHE:N	2.34	0.42
1:E:328:PRO:HD2	1:E:392:ARG:HG2	2.01	0.42
1:D:470:ARG:CZ	1:D:514:ILE:HD11	2.50	0.42
1:A:302:MET:CE	1:A:359:TYR:CE2	3.02	0.42
1:B:398:THR:O	1:B:398:THR:CG2	2.67	0.42
1:F:368:ASN:O	1:F:369:SER:HB2	2.19	0.42
1:D:502:LYS:HG2	1:D:503:VAL:N	2.34	0.42
1:F:466:SER:CB	1:F:517:CYS:O	2.64	0.42
1:A:273:PRO:HB3	1:A:456:ILE:HG22	2.02	0.42
1:D:511:ASP:OD1	1:D:512:ASN:N	2.52	0.42
1:D:302:MET:HE3	1:D:302:MET:HB2	1.94	0.42
1:C:346:MET:HB3	1:C:346:MET:HE3	1.86	0.42
1:E:233:LEU:HD12	1:E:346:MET:HB3	2.02	0.42
1:G:420:THR:HA	1:G:423:LYS:HE2	2.01	0.42
1:G:325:LEU:HD23	1:G:325:LEU:HA	1.89	0.42
1:G:354:GLN:HG3	1:G:355:ALA:N	2.34	0.42
1:D:390:SER:HB3	1:D:391:PRO:HD3	2.01	0.42
1:A:425:LEU:HD22	1:A:555:LYS:HE3	2.02	0.42
1:C:488:LEU:HB2	1:C:490:TYR:HE2	1.85	0.42
1:A:543:MET:HE2	1:A:543:MET:HB3	1.88	0.42
1:B:236:VAL:CG2	1:B:355:ALA:HB3	2.50	0.42
1:F:527:MET:HG3	1:F:528:ARG:H	1.85	0.42
1:A:510:TYR:CD1	1:A:529:GLN:HB2	2.55	0.42
1:D:503:VAL:HG12	1:D:508:LYS:HE2	2.02	0.42
1:B:363:ASP:OD1	1:B:448:TYR:CD1	2.73	0.42
1:C:511:ASP:C	1:C:513:LYS:H	2.24	0.42
1:B:244:VAL:HG12	1:B:250:LEU:HB2	2.01	0.42
1:D:344:GLY:HA3	1:D:360:LEU:O	2.20	0.42
1:A:385:GLU:HG2	1:A:412:ASN:HD21	1.85	0.42
1:F:419:CYS:O	1:F:422:ARG:HB2	2.20	0.41
1:B:491:VAL:CG2	1:B:498:PHE:HB2	2.50	0.41
1:B:279:GLN:O	1:B:282:LYS:HB2	2.20	0.41
1:F:507:LEU:HD23	1:F:507:LEU:N	2.35	0.41
1:A:539:TYR:CD2	1:A:539:TYR:C	2.94	0.41
1:A:530:ARG:CG	1:A:530:ARG:NH1	2.83	0.41
1:G:277:ASP:HB2	1:G:551:ASN:OD1	2.21	0.41
1:F:468:ASP:HB2	1:F:537:ASN:ND2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:VAL:HG21	1:F:469:PHE:HE1	1.81	0.41
1:E:545:VAL:O	1:E:549:ILE:HG13	2.19	0.41
1:E:361:ILE:CG2	1:E:384:ILE:HD13	2.48	0.41
1:D:440:LEU:HA	1:D:440:LEU:HD23	1.85	0.41
1:D:516:GLU:HG2	1:D:527:MET:CG	2.50	0.41
1:E:402:ASP:O	1:E:405:GLN:HG2	2.19	0.41
1:F:374:ASP:OD2	1:F:447:LYS:HE3	2.20	0.41
1:C:282:LYS:HE2	1:C:282:LYS:HB3	1.89	0.41
1:B:264:GLU:HA	1:B:264:GLU:OE2	2.20	0.41
1:A:286:LEU:HD13	1:D:519:PHE:CE1	2.39	0.41
1:A:422:ARG:HB3	1:A:562:ILE:HG22	2.01	0.41
1:E:377:PHE:CE2	1:E:381:LEU:HD22	2.56	0.41
1:A:291:VAL:HG11	1:A:421:SER:HB2	2.01	0.41
1:D:488:LEU:HB2	1:D:490:TYR:CE2	2.55	0.41
1:E:521:ASN:O	1:E:522:ASN:CB	2.69	0.41
1:B:325:LEU:HD13	1:B:327:PHE:CZ	2.56	0.41
1:G:521:ASN:O	1:G:522:ASN:OD1	2.39	0.41
1:B:443:GLN:HA	1:B:444:PRO:HD2	1.82	0.41
1:D:484:GLN:HG2	1:D:485:ASN:N	2.35	0.41
1:B:259:GLN:O	1:F:521:ASN:ND2	2.53	0.41
1:E:321:HIS:HE1	1:E:323:SER:HA	1.86	0.41
1:A:370:GLN:O	1:A:372:VAL:N	2.53	0.41
1:G:438:ASP:O	1:G:460:LYS:HG3	2.20	0.41
1:E:489:LEU:HD22	1:E:515:ILE:HD11	2.03	0.41
1:B:291:VAL:CG2	1:B:440:LEU:HD13	2.48	0.41
1:A:287:LYS:HA	1:D:498:PHE:O	2.20	0.41
1:C:312:MET:O	1:C:319:VAL:HA	2.20	0.41
1:A:410:VAL:HG12	1:A:410:VAL:O	2.18	0.41
1:C:298:THR:HG23	1:C:315:ARG:HH22	1.84	0.41
1:B:232:PHE:HB2	1:B:320:PHE:CZ	2.54	0.41
1:B:494:TYR:CZ	1:B:496:ARG:HB2	2.55	0.41
1:G:467:VAL:CG1	1:G:469:PHE:CE2	3.03	0.41
1:F:311:PHE:HA	1:F:320:PHE:O	2.21	0.41
1:B:386:ARG:HH11	1:B:386:ARG:HB2	1.84	0.41
1:F:377:PHE:HD1	1:F:380:ARG:HH21	1.67	0.41
1:C:377:PHE:CE2	1:C:443:GLN:HG2	2.56	0.41
1:C:335:MET:HE3	1:C:335:MET:HA	2.02	0.41
1:D:247:GLN:N	1:D:248:PRO:HD2	2.36	0.41
1:F:508:LYS:HE3	1:F:508:LYS:HB2	1.70	0.41
1:F:467:VAL:CG1	1:F:545:VAL:HG11	2.50	0.41
1:D:358:ARG:HB2	1:D:358:ARG:HE	1.66	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:527:MET:HE2	1:F:528:ARG:HG2	2.02	0.41
1:G:276:MET:HG3	1:G:457:LEU:HD13	2.01	0.41
1:C:233:LEU:HD11	1:C:348:ILE:HG13	2.03	0.41
1:G:520:GLU:CG	1:G:525:VAL:HG11	2.50	0.41
1:B:290:LYS:NZ	1:B:417:ASP:HB3	2.36	0.41
1:F:279:GLN:O	1:F:282:LYS:HB2	2.21	0.41
1:E:325:LEU:HD12	1:E:406:GLU:OE2	2.21	0.41
1:B:263:TRP:CH2	1:B:451:GLY:HA3	2.55	0.41
1:G:381:LEU:HD23	1:G:381:LEU:HA	1.91	0.41
1:D:328:PRO:HG3	1:D:395:LYS:HD2	2.02	0.41
1:E:461:PRO:HA	1:E:462:PRO:HD3	1.95	0.41
1:E:358:ARG:HE	1:E:358:ARG:HB2	1.61	0.41
1:E:358:ARG:NH1	1:E:411:ARG:CZ	2.83	0.41
1:A:435:HIS:CD2	1:A:436:GLU:H	2.39	0.41
1:A:435:HIS:CE1	1:A:436:GLU:HB2	2.56	0.41
1:B:324:ASN:O	1:B:406:GLU:HG2	2.21	0.41
1:E:376:ASP:O	1:E:379:VAL:HB	2.20	0.41
1:D:498:PHE:CZ	1:D:542:ALA:HB1	2.55	0.41
1:C:325:LEU:HA	1:C:325:LEU:HD23	1.92	0.41
1:F:274:VAL:HG21	1:F:454:ASP:HA	2.02	0.41
1:F:304:ILE:HB	1:F:340:THR:HB	2.03	0.41
1:D:364:ILE:O	1:D:364:ILE:HG23	2.21	0.41
1:F:514:ILE:HD12	1:F:514:ILE:N	2.36	0.41
1:G:321:HIS:C	1:G:321:HIS:ND1	2.74	0.41
1:G:244:VAL:HB	1:G:319:VAL:HG22	2.03	0.41
1:E:503:VAL:HA	1:E:507:LEU:HD22	2.03	0.40
1:B:499:ALA:HB1	1:B:524:TRP:CD1	2.56	0.40
1:E:314:ASP:C	1:E:316:ASP:N	2.73	0.40
1:E:333:LEU:O	1:E:395:LYS:HE3	2.20	0.40
1:C:498:PHE:CE1	1:C:542:ALA:HB1	2.56	0.40
1:F:287:LYS:HB2	1:F:288:PRO:HD2	2.03	0.40
1:G:494:TYR:HD1	1:G:496:ARG:O	2.04	0.40
1:F:545:VAL:O	1:F:548:SER:HB2	2.22	0.40
1:C:560:GLU:HA	1:C:563:ASP:CB	2.44	0.40
1:F:526:PHE:CZ	1:F:528:ARG:O	2.75	0.40
1:A:420:THR:HG22	1:A:420:THR:O	2.21	0.40
1:F:346:MET:CE	1:F:359:TYR:CD1	3.04	0.40
1:C:237:THR:O	1:C:237:THR:HG22	2.21	0.40
1:G:341:LEU:HD23	1:G:365:ILE:CB	2.50	0.40
1:F:329:PHE:CE2	1:F:331:LYS:CG	3.04	0.40
1:C:304:ILE:HD13	1:C:327:PHE:CD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:GLU:HA	1:C:407:PRO:HD3	1.67	0.40
1:B:406:GLU:HA	1:B:407:PRO:HD3	1.86	0.40
1:C:555:LYS:HD2	1:C:555:LYS:H	1.87	0.40
1:G:494:TYR:CE2	1:G:539:TYR:CE1	3.09	0.40
1:C:515:ILE:HB	1:C:526:PHE:HE1	1.86	0.40
1:F:449:LYS:HA	1:F:450:PRO:HD3	1.77	0.40
1:G:332:ASP:HB3	1:G:335:MET:HE3	2.04	0.40
1:G:505:LYS:HG2	1:G:505:LYS:H	1.59	0.40
1:B:278:LYS:O	1:B:281:ILE:HG22	2.22	0.40
1:A:513:LYS:HE2	1:A:529:GLN:HE22	1.87	0.40
1:A:530:ARG:HG3	1:A:532:ASP:OD1	2.22	0.40
1:A:319:VAL:HG12	1:A:320:PHE:N	2.37	0.40
1:D:449:LYS:HA	1:D:450:PRO:HD2	1.86	0.40
1:F:361:ILE:HG22	1:F:384:ILE:HD13	2.02	0.40
1:D:368:ASN:O	1:D:369:SER:HB2	2.22	0.40
1:F:392:ARG:NH2	1:F:406:GLU:OE1	2.55	0.40
1:F:316:ASP:O	1:F:317:ASN:CB	2.69	0.40
1:G:462:PRO:O	1:G:465:ASN:HB2	2.21	0.40
1:F:243:GLN:HG2	1:F:244:VAL:N	2.37	0.40
1:G:377:PHE:CD2	1:G:443:GLN:HG2	2.56	0.40
1:A:482:LEU:HD22	1:A:483:PRO:HD2	2.02	0.40
1:B:285:ASP:OD1	1:B:561:PHE:HE2	2.05	0.40
1:E:489:LEU:HD11	1:E:501:ILE:HB	2.04	0.40
1:B:289:TYR:O	1:B:418:ILE:HG13	2.21	0.40
1:G:491:VAL:HG22	1:G:539:TYR:HA	2.03	0.40
1:E:367:PHE:O	1:E:368:ASN:HB2	2.21	0.40
1:C:402:ASP:OD2	1:C:405:GLN:HG2	2.22	0.40
1:C:564:ARG:HH11	1:F:486:VAL:HG21	1.86	0.40
1:F:396:MET:HG3	1:F:401:ILE:CG2	2.52	0.40
1:B:554:THR:C	1:B:556:GLU:N	2.74	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	324/347 (93%)	313 (97%)	11 (3%)	0	100 100
1	B	310/347 (89%)	291 (94%)	18 (6%)	1 (0%)	46 82
1	C	308/347 (89%)	296 (96%)	11 (4%)	1 (0%)	46 82
1	D	324/347 (93%)	313 (97%)	11 (3%)	0	100 100
1	E	325/347 (94%)	308 (95%)	17 (5%)	0	100 100
1	F	329/347 (95%)	312 (95%)	17 (5%)	0	100 100
1	G	325/347 (94%)	307 (94%)	18 (6%)	0	100 100
All	All	2245/2429 (92%)	2140 (95%)	103 (5%)	2 (0%)	56 90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	VAL
1	C	232	PHE

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	296/313 (95%)	255 (86%)	41 (14%)	4 19
1	B	288/313 (92%)	250 (87%)	38 (13%)	5 21
1	C	286/313 (91%)	258 (90%)	28 (10%)	10 35
1	D	296/313 (95%)	267 (90%)	29 (10%)	10 35
1	E	297/313 (95%)	276 (93%)	21 (7%)	18 53
1	F	294/313 (94%)	273 (93%)	21 (7%)	18 53
1	G	296/313 (95%)	262 (88%)	34 (12%)	7 27
All	All	2053/2191 (94%)	1841 (90%)	212 (10%)	9 32

All (212) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	LEU
1	A	236	VAL
1	A	239	LYS
1	A	250	LEU
1	A	258	HIS
1	A	266	SER
1	A	275	SER
1	A	283	LEU
1	A	307	THR
1	A	308	ASN
1	A	316	ASP
1	A	322	VAL
1	A	326	GLU
1	A	329	PHE
1	A	335	MET
1	A	348	ILE
1	A	349	ASP
1	A	358	ARG
1	A	362	TYR
1	A	369	SER
1	A	378	ASN
1	A	381	LEU
1	A	383	CYS
1	A	386	ARG
1	A	389	ILE
1	A	390	SER
1	A	416	PHE
1	A	418	ILE
1	A	419	CYS
1	A	441	ILE
1	A	457	LEU
1	A	460	LYS
1	A	463	SER
1	A	471	LEU
1	A	479	GLU
1	A	481	LEU
1	A	495	GLU
1	A	510	TYR
1	A	525	VAL
1	A	528	ARG
1	A	530	ARG
1	B	245	THR
1	B	250	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	264	GLU
1	B	266	SER
1	B	283	LEU
1	B	293	TRP
1	B	319	VAL
1	B	323	SER
1	B	326	GLU
1	B	329	PHE
1	B	338	SER
1	B	348	ILE
1	B	349	ASP
1	B	352	ASN
1	B	356	VAL
1	B	360	LEU
1	B	362	TYR
1	B	368	ASN
1	B	370	GLN
1	B	378	ASN
1	B	389	ILE
1	B	390	SER
1	B	396	MET
1	B	409	SER
1	B	416	PHE
1	B	418	ILE
1	B	420	THR
1	B	440	LEU
1	B	441	ILE
1	B	468	ASP
1	B	471	LEU
1	B	491	VAL
1	B	510	TYR
1	B	523	SER
1	B	529	GLN
1	B	543	MET
1	B	555	LYS
1	B	559	PHE
1	C	233	LEU
1	C	237	THR
1	C	275	SER
1	C	293	TRP
1	C	298	THR
1	C	312	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	323	SER
1	C	326	GLU
1	C	336	HIS
1	C	362	TYR
1	C	368	ASN
1	C	378	ASN
1	C	390	SER
1	C	408	PHE
1	C	416	PHE
1	C	425	LEU
1	C	435	HIS
1	C	443	GLN
1	C	445	THR
1	C	457	LEU
1	C	488	LEU
1	C	498	PHE
1	C	505	LYS
1	C	529	GLN
1	C	532	ASP
1	C	537	ASN
1	C	548	SER
1	C	563	ASP
1	D	239	LYS
1	D	242	THR
1	D	244	VAL
1	D	245	THR
1	D	293	TRP
1	D	316	ASP
1	D	318	SER
1	D	329	PHE
1	D	351	VAL
1	D	362	TYR
1	D	376	ASP
1	D	381	LEU
1	D	389	ILE
1	D	409	SER
1	D	419	CYS
1	D	421	SER
1	D	441	ILE
1	D	452	ARG
1	D	453	CYS
1	D	464	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	470	ARG
1	D	506	GLU
1	D	507	LEU
1	D	521	ASN
1	D	531	THR
1	D	548	SER
1	D	554	THR
1	D	559	PHE
1	D	564	ARG
1	E	286	LEU
1	E	293	TRP
1	E	308	ASN
1	E	309	GLU
1	E	314	ASP
1	E	362	TYR
1	E	366	LYS
1	E	381	LEU
1	E	390	SER
1	E	409	SER
1	E	418	ILE
1	E	425	LEU
1	E	447	LYS
1	E	452	ARG
1	E	464	LEU
1	E	514	ILE
1	E	518	LYS
1	E	543	MET
1	E	556	GLU
1	E	563	ASP
1	E	565	CYS
1	G	231	ILE
1	G	250	LEU
1	G	293	TRP
1	G	307	THR
1	G	317	ASN
1	G	321	HIS
1	G	329	PHE
1	G	362	TYR
1	G	376	ASP
1	G	378	ASN
1	G	389	ILE
1	G	405	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	409	SER
1	G	411	ARG
1	G	413	LYS
1	G	420	THR
1	G	441	ILE
1	G	458	LYS
1	G	464	LEU
1	G	466	SER
1	G	476	MET
1	G	485	ASN
1	G	489	LEU
1	G	496	ARG
1	G	510	TYR
1	G	512	ASN
1	G	521	ASN
1	G	522	ASN
1	G	526	PHE
1	G	528	ARG
1	G	530	ARG
1	G	532	ASP
1	G	549	ILE
1	G	555	LYS
1	F	237	THR
1	F	239	LYS
1	F	244	VAL
1	F	250	LEU
1	F	293	TRP
1	F	329	PHE
1	F	347	ILE
1	F	362	TYR
1	F	378	ASN
1	F	398	THR
1	F	409	SER
1	F	413	LYS
1	F	416	PHE
1	F	425	LEU
1	F	441	ILE
1	F	463	SER
1	F	467	VAL
1	F	516	GLU
1	F	537	ASN
1	F	555	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	557	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	243	GLN
1	A	280	ASN
1	A	412	ASN
1	A	435	HIS
1	A	521	ASN
1	B	280	ASN
1	B	412	ASN
1	C	280	ASN
1	C	412	ASN
1	C	435	HIS
1	D	280	ASN
1	D	529	GLN
1	E	280	ASN
1	E	393	HIS
1	G	280	ASN
1	G	435	HIS
1	G	529	GLN
1	F	280	ASN
1	F	537	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	1	-	4,4,4	0.14	0	6,6,6	0.37	0
2	SO4	A	2	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	A	3	-	4,4,4	0.36	0	6,6,6	0.29	0
2	SO4	A	5	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	B	4	-	4,4,4	0.17	0	6,6,6	0.44	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
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	A	5	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	SO4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	328/347 (94%)	0.32	17 (5%) 31 12	28, 51, 102, 136	0
1	B	316/347 (91%)	0.65	45 (14%) 4 1	29, 67, 127, 137	0
1	C	314/347 (90%)	0.46	31 (9%) 9 3	26, 59, 121, 135	0
1	D	328/347 (94%)	0.31	20 (6%) 25 9	28, 55, 112, 143	0
1	E	329/347 (94%)	0.59	37 (11%) 7 2	22, 59, 128, 144	0
1	F	333/347 (95%)	0.32	20 (6%) 25 9	23, 52, 119, 148	0
1	G	329/347 (94%)	0.42	33 (10%) 9 3	30, 61, 127, 149	0
All	All	2277/2429 (93%)	0.44	203 (8%) 12 4	22, 57, 123, 149	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	526	PHE	8.3
1	B	504	THR	7.6
1	E	512	ASN	7.4
1	A	564	ARG	7.3
1	G	483	PRO	7.0
1	C	503	VAL	6.8
1	D	482	LEU	6.7
1	E	477	GLY	6.7
1	A	400	LEU	6.7
1	F	477	GLY	6.5
1	E	481	LEU	6.3
1	C	509	GLN	5.9
1	F	504	THR	5.9
1	B	473	ILE	5.9
1	B	507	LEU	5.8
1	G	503	VAL	5.7
1	D	481	LEU	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	481	LEU	5.6
1	B	355	ALA	5.5
1	G	424	LEU	5.5
1	B	471	LEU	5.4
1	G	481	LEU	5.1
1	F	486	VAL	4.9
1	C	490	TYR	4.9
1	C	493	GLY	4.9
1	E	230	ALA	4.8
1	E	486	VAL	4.7
1	E	478	GLY	4.6
1	E	531	THR	4.5
1	E	487	GLY	4.5
1	G	482	LEU	4.5
1	A	401	ILE	4.5
1	B	470	ARG	4.4
1	G	477	GLY	4.4
1	C	352	ASN	4.3
1	B	229	GLY	4.3
1	B	527	MET	4.3
1	E	509	GLN	4.3
1	G	479	GLU	4.3
1	B	509	GLN	4.2
1	D	480	GLY	4.2
1	G	437	MET	4.1
1	E	510	TYR	4.0
1	G	502	LYS	4.0
1	G	435	HIS	4.0
1	A	398	THR	4.0
1	B	350	ARG	4.0
1	A	399	GLY	4.0
1	E	422	ARG	3.9
1	B	503	VAL	3.9
1	G	510	TYR	3.9
1	F	482	LEU	3.9
1	D	424	LEU	3.9
1	A	353	GLY	3.9
1	B	511	ASP	3.8
1	C	507	LEU	3.8
1	C	564	ARG	3.8
1	D	425	LEU	3.8
1	F	478	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	503	VAL	3.8
1	G	509	GLN	3.7
1	B	420	THR	3.7
1	F	483	PRO	3.7
1	G	421	SER	3.6
1	C	424	LEU	3.6
1	E	507	LEU	3.6
1	G	352	ASN	3.6
1	B	235	GLY	3.6
1	D	564	ARG	3.6
1	C	515	ILE	3.5
1	A	336	HIS	3.5
1	B	230	ALA	3.5
1	E	421	SER	3.4
1	A	403	LYS	3.4
1	F	513	LYS	3.4
1	E	352	ASN	3.4
1	B	533	LYS	3.4
1	F	535	PHE	3.3
1	G	504	THR	3.3
1	E	476	MET	3.3
1	B	529	GLN	3.3
1	B	234	GLU	3.3
1	C	498	PHE	3.3
1	E	470	ARG	3.3
1	B	472	LYS	3.3
1	B	352	ASN	3.3
1	G	420	THR	3.3
1	B	512	ASN	3.3
1	F	487	GLY	3.2
1	E	504	THR	3.2
1	C	506	GLU	3.2
1	C	470	ARG	3.2
1	G	485	ASN	3.2
1	A	481	LEU	3.1
1	D	478	GLY	3.1
1	A	394	GLU	3.1
1	B	535	PHE	3.1
1	D	485	ASN	3.1
1	E	505	LYS	3.1
1	B	348	ILE	3.0
1	G	422	ARG	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	506	GLU	3.0
1	E	526	PHE	3.0
1	D	535	PHE	2.9
1	B	514	ILE	2.9
1	D	423	LYS	2.9
1	E	471	LEU	2.9
1	G	478	GLY	2.9
1	F	514	ILE	2.9
1	C	494	TYR	2.9
1	D	265	GLY	2.9
1	C	469	PHE	2.8
1	B	422	ARG	2.8
1	E	479	GLU	2.8
1	B	530	ARG	2.8
1	E	474	THR	2.8
1	B	491	VAL	2.8
1	E	355	ALA	2.8
1	C	435	HIS	2.8
1	D	479	GLU	2.7
1	E	475	ARG	2.7
1	B	353	GLY	2.7
1	G	526	PHE	2.7
1	B	351	VAL	2.7
1	F	503	VAL	2.7
1	A	396	MET	2.7
1	A	352	ASN	2.6
1	G	506	GLU	2.6
1	B	548	SER	2.6
1	C	502	LYS	2.6
1	E	529	GLN	2.6
1	G	471	LEU	2.6
1	B	508	LYS	2.6
1	F	506	GLU	2.6
1	C	421	SER	2.6
1	B	486	VAL	2.6
1	B	534	SER	2.6
1	C	488	LEU	2.6
1	F	480	GLY	2.6
1	A	483	PRO	2.6
1	C	436	GLU	2.6
1	E	488	LEU	2.6
1	G	490	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	266	SER	2.5
1	C	513	LYS	2.5
1	D	421	SER	2.5
1	E	490	TYR	2.5
1	D	483	PRO	2.5
1	E	508	LYS	2.5
1	C	487	GLY	2.4
1	G	562	ILE	2.4
1	G	293	TRP	2.4
1	C	501	ILE	2.4
1	E	496	ARG	2.4
1	B	233	LEU	2.4
1	B	564	ARG	2.4
1	C	422	ARG	2.4
1	D	476	MET	2.4
1	B	398	THR	2.4
1	E	491	VAL	2.4
1	A	351	VAL	2.4
1	B	236	VAL	2.4
1	B	517	CYS	2.3
1	F	479	GLU	2.3
1	B	334	ARG	2.3
1	C	528	ARG	2.3
1	F	505	LYS	2.3
1	E	480	GLY	2.3
1	C	425	LEU	2.3
1	B	510	TYR	2.3
1	E	317	ASN	2.3
1	G	505	LYS	2.3
1	A	354	GLN	2.3
1	F	509	GLN	2.3
1	G	493	GLY	2.3
1	A	239	LYS	2.3
1	C	437	MET	2.2
1	A	402	ASP	2.2
1	B	515	ILE	2.2
1	C	354	GLN	2.2
1	G	473	ILE	2.2
1	F	352	ASN	2.2
1	C	403	LYS	2.2
1	G	236	VAL	2.2
1	C	531	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	492	GLY	2.2
1	G	480	GLY	2.1
1	B	349	ASP	2.1
1	E	308	ASN	2.1
1	G	351	VAL	2.1
1	F	501	ILE	2.1
1	D	559	PHE	2.1
1	G	527	MET	2.1
1	C	562	ILE	2.1
1	B	232	PHE	2.1
1	D	354	GLN	2.0
1	E	473	ILE	2.0
1	D	237	THR	2.0
1	D	250	LEU	2.0
1	B	559	PHE	2.0
1	D	563	ASP	2.0
1	G	309	GLU	2.0
1	F	247	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	3	5/5	0.98	0.28	0.97	41,46,53,55	0
2	SO4	A	5	5/5	0.91	0.22	-0.70	72,75,93,93	0
2	SO4	A	2	5/5	0.96	0.12	-5.12	47,58,60,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	A	1	5/5	0.84	0.27	-	68,72,86,94	0
2	SO4	B	4	5/5	0.90	0.18	-	75,79,82,89	0

6.5 Other polymers (i)

There are no such residues in this entry.