



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:58 pm BST

PDB ID : 1ZM2  
Title : Structure of ADP-ribosylated eEF2 in complex with catalytic fragment of ETA  
Authors : Joergensen, R.; Merrill, A.R.; Yates, S.P.; Marquez, V.E.; Schwan, A.L.; Boesen, T.; Andersen, G.R.  
Deposited on : 2005-05-10  
Resolution : 3.07 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](mailto: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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

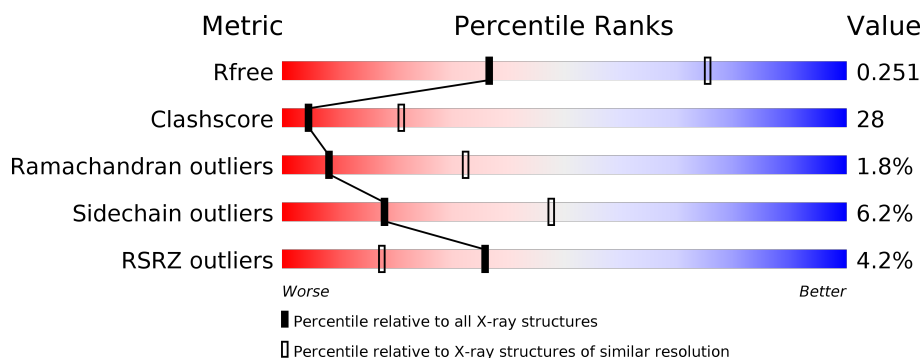
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.07 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	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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  $\geq 3$ , 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	842	
1	C	842	
1	E	842	
2	B	207	
2	D	207	
2	F	207	

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
1	DDE	E	699	-	-	X	-
3	APR	E	843	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24024 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	C	823	Total	C	N	O	S	0	0	0
			6405	4075	1093	1207	30			
1	E	823	Total	C	N	O	S	0	0	0
			6415	4082	1095	1208	30			

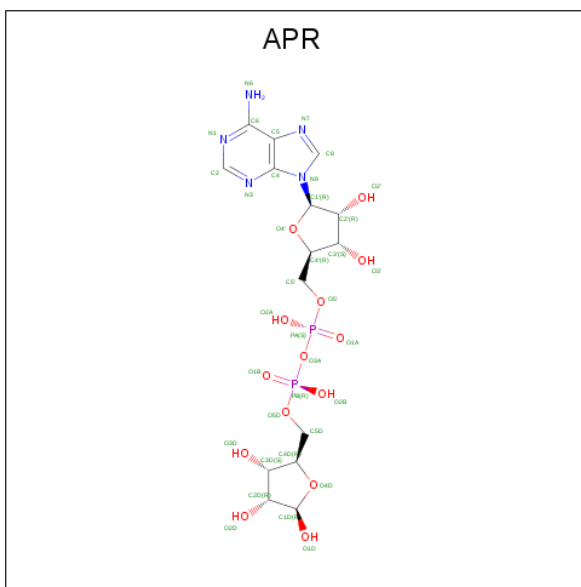
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
C	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324
E	699	DDE	HIS	MODIFIED RESIDUE	UNP P32324

- Molecule 2 is a protein called Exotoxin A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	D	207	Total	C	N	O	0	0	0
			1588	1001	283	304			
2	F	207	Total	C	N	O	0	0	0
			1588	1001	283	304			

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>14</sub>P<sub>2</sub>).

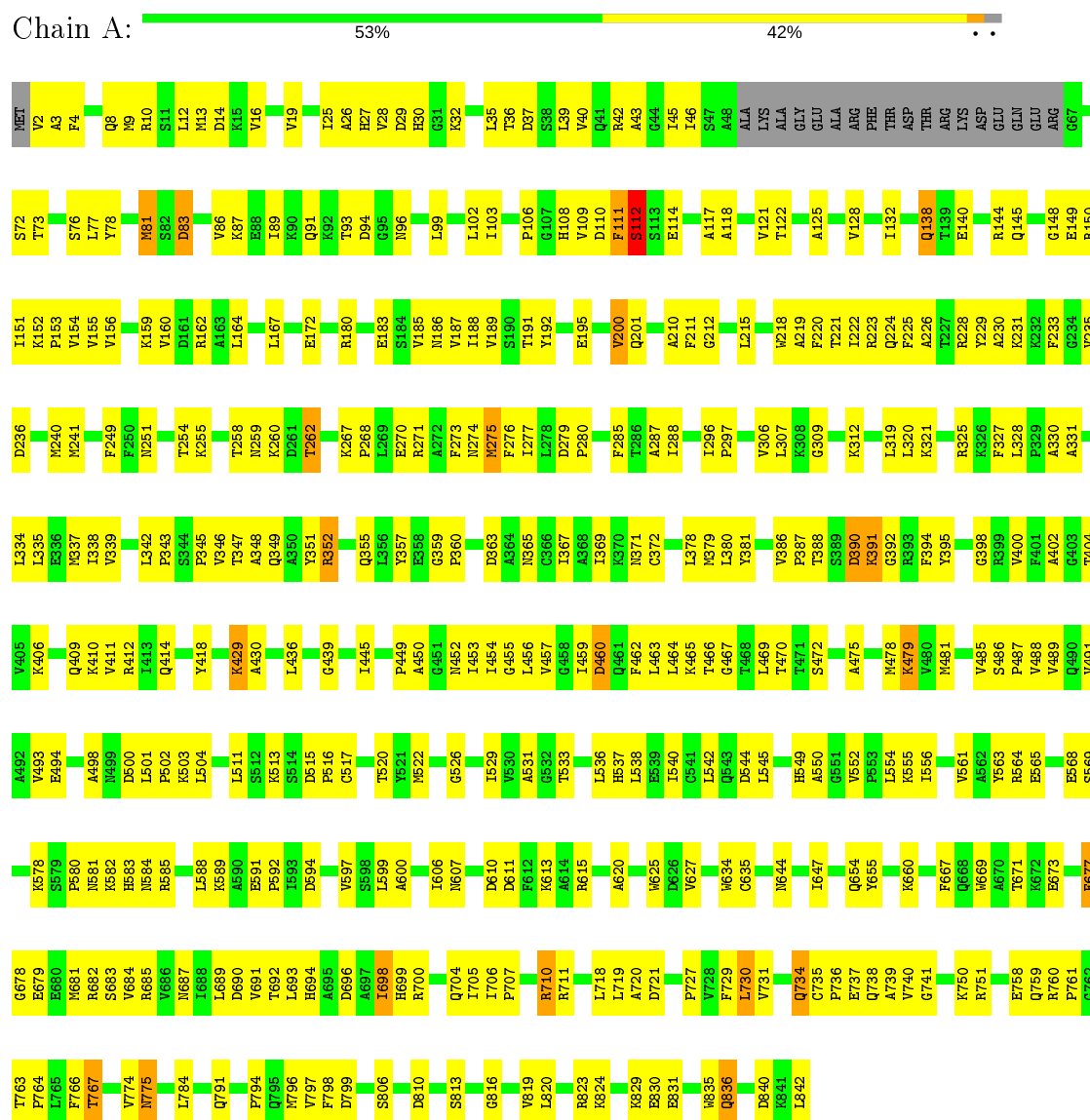


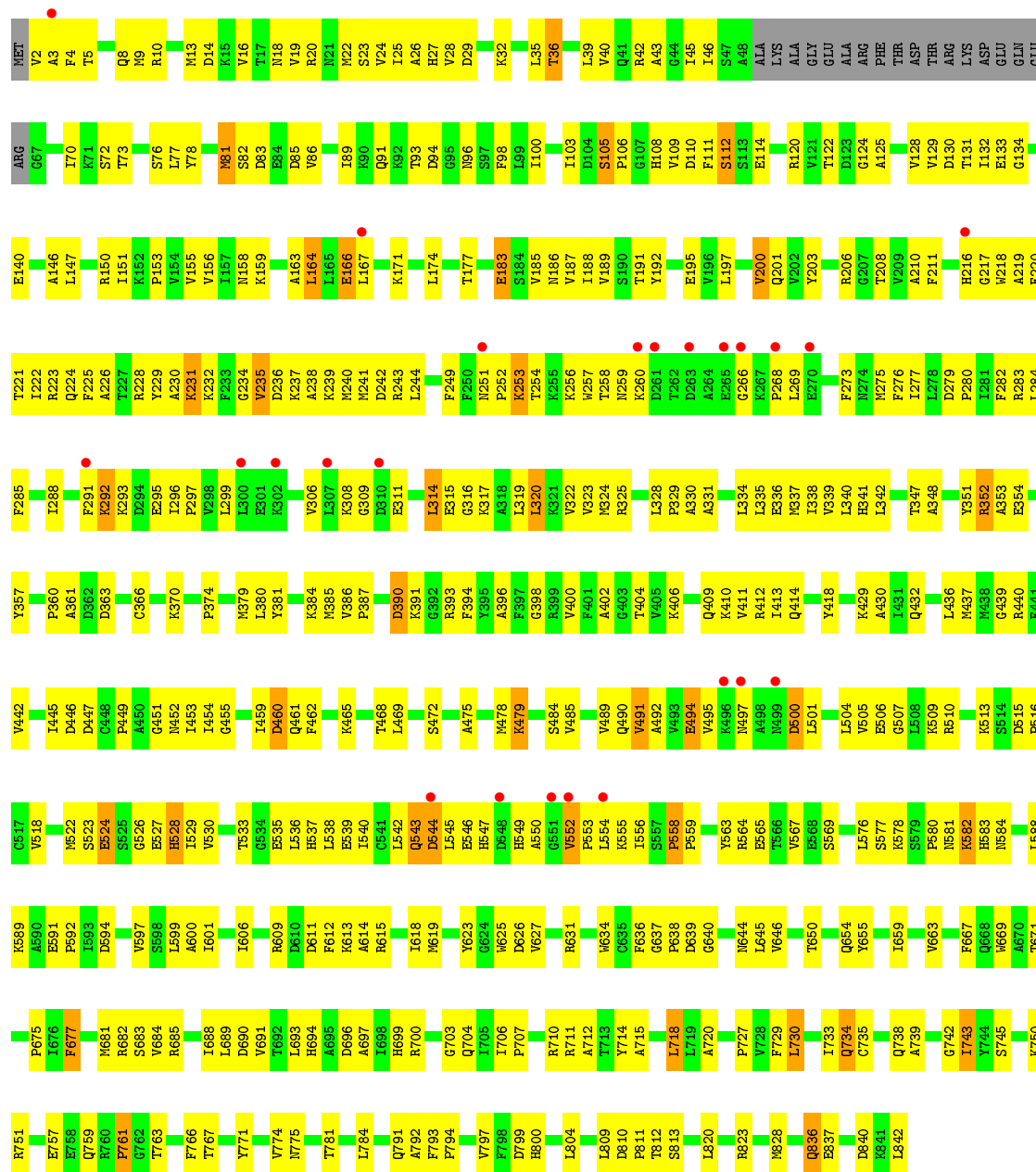
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Elongation factor 2

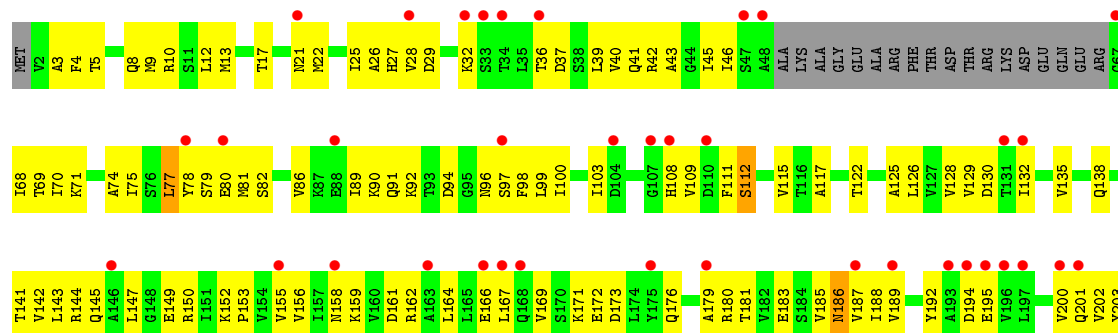


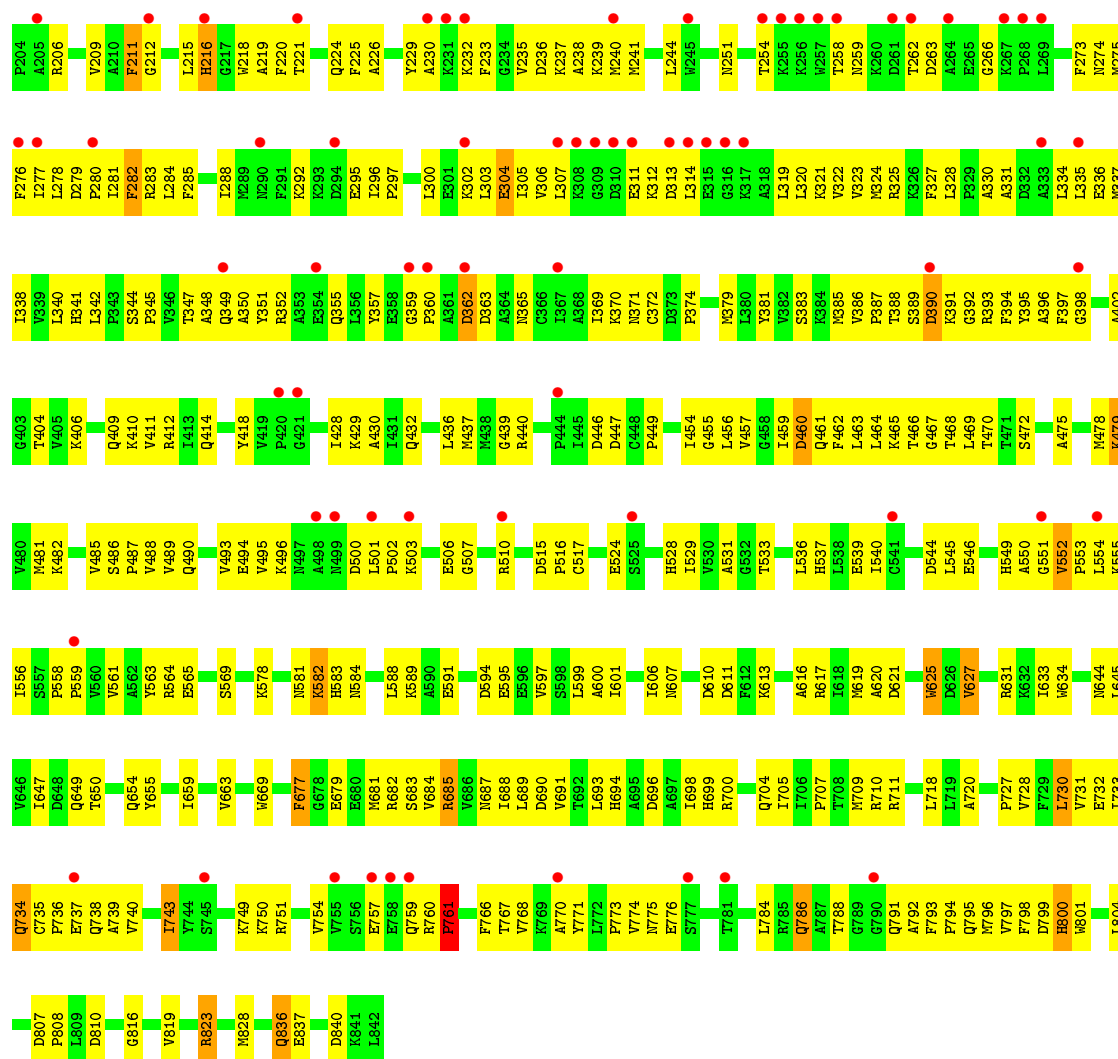


- Molecule 1: Elongation factor 2



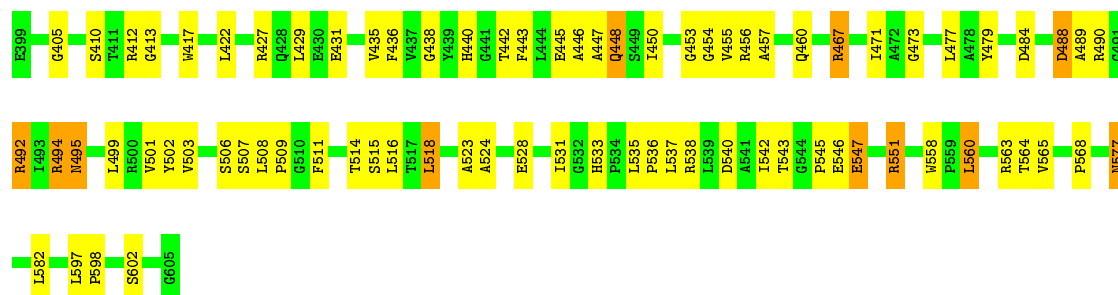
Chain E:





● Molecule 2: Exotoxin A

Chain B: 62% 32% 5%

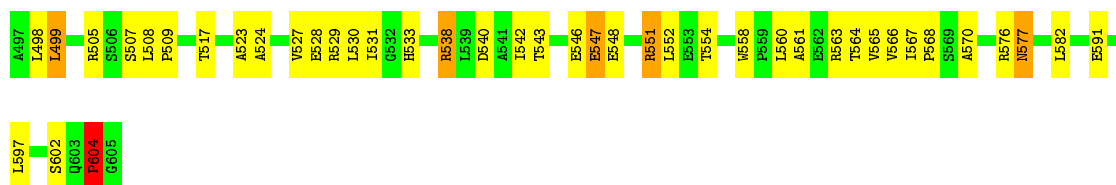


● Molecule 2: Exotoxin A

Chain D: 59% 35% 5%

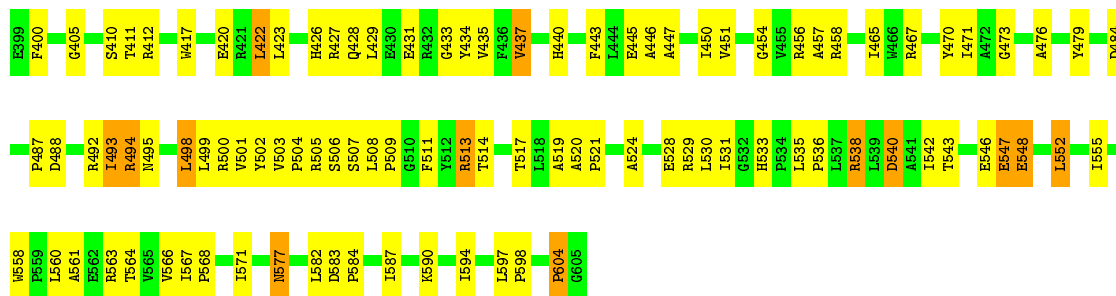






• Molecule 2: Exotoxin A

Chain F: 53% 41% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	330.63Å 67.84Å 191.50Å 90.00° 103.30° 90.00°	Depositor
Resolution (Å)	30.00 – 3.07 29.63 – 3.07	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.07) 99.4 (29.63-3.07)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.06Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.231 , 0.265 0.224 , 0.251	Depositor DCC
$R_{free}$ test set	1552 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	24024	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0079e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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

### 5.1 Standard geometry

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

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	0.47	0/6517	0.68	0/8823
1	C	0.43	0/6517	0.67	0/8823
1	E	0.41	0/6517	0.64	0/8823
2	B	0.60	0/1627	0.86	0/2216
2	D	0.58	0/1627	0.81	0/2216
2	F	0.57	0/1627	0.84	1/2216 (0.0%)
All	All	0.47	0/24432	0.70	1/33117 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	494	ARG	NE-CZ-NH1	6.14	123.37	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	6405	0	6472	342	0
1	C	6405	0	6472	377	0
1	E	6415	0	6487	422	0
2	B	1588	0	1539	66	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1588	0	1539	74	0
2	F	1588	0	1539	82	0
3	E	35	0	19	6	0
All	All	24024	0	24067	1350	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 28.

All (1350) 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)
2:D:546:GLU:HG3	2:D:547:GLU:HG3	1.29	1.14
2:B:546:GLU:HG3	2:B:547:GLU:HG3	1.32	1.11
1:C:404:THR:HG22	1:C:449:PRO:HA	1.34	1.05
1:E:68:ILE:HD12	1:E:390:ASP:HB2	1.37	1.03
1:C:231:LYS:HE3	1:C:232:LYS:HG3	1.42	1.02
1:C:253:LYS:HE3	1:C:253:LYS:HA	1.41	1.01
1:E:71:LYS:HE3	1:E:387:PRO:HD2	1.41	1.01
2:D:488:ASP:OD2	2:D:490:ARG:HG2	1.60	1.01
1:C:256:LYS:HD3	1:C:257:TRP:H	1.25	0.99
2:B:455:VAL:O	2:B:456:ARG:HD2	1.63	0.99
1:A:45:ILE:HD11	1:A:78:TYR:HB2	1.45	0.97
1:E:77:LEU:HB2	1:E:100:ILE:HB	1.47	0.96
1:A:737:GLU:HG3	1:A:766:PHE:CE2	2.00	0.96
2:F:546:GLU:HG3	2:F:547:GLU:HG3	1.44	0.95
1:E:91:GLN:HE22	1:E:344:SER:H	1.13	0.94
1:C:315:GLU:HA	1:C:319:LEU:HB2	1.48	0.94
1:A:694:HIS:HD2	1:A:696:ASP:H	1.15	0.94
1:A:627:VAL:HG12	2:F:405:GLY:HA2	1.50	0.93
1:C:552:VAL:HG22	1:C:553:PRO:HD2	1.49	0.93
2:F:513:ARG:HH11	2:F:513:ARG:HB2	1.34	0.92
1:E:694:HIS:HD2	1:E:696:ASP:H	1.11	0.90
1:A:737:GLU:HG3	1:A:766:PHE:HE2	1.35	0.90
1:E:147:LEU:HD13	1:E:192:TYR:HB2	1.53	0.90
1:A:409:GLN:HE21	1:A:411:VAL:HG22	1.37	0.89
1:A:731:VAL:HG12	1:A:796:MET:HB3	1.56	0.88
1:E:155:VAL:HG23	1:E:202:VAL:HG11	1.56	0.88
1:C:42:ARG:HG3	1:C:331:ALA:CB	2.04	0.87
1:A:258:THR:HG22	1:A:259:ASN:H	1.39	0.87
1:E:545:LEU:HD12	1:E:549:HIS:HB2	1.56	0.86
1:A:710:ARG:HG3	1:A:710:ARG:HH11	1.42	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:HIS:HD2	1:C:29:ASP:H	1.24	0.85
1:A:404:THR:HG22	1:A:449:PRO:HA	1.58	0.85
1:E:45:ILE:HD11	1:E:78:TYR:CB	2.07	0.85
2:B:495:ASN:N	2:B:495:ASN:HD22	1.73	0.84
1:E:45:ILE:HD11	1:E:78:TYR:HB2	1.57	0.84
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.59	0.84
1:A:533:THR:H	1:A:537:HIS:CD2	1.95	0.83
1:A:533:THR:H	1:A:537:HIS:HD2	1.25	0.83
2:B:537:LEU:O	2:B:538:ARG:HD3	1.77	0.83
1:E:27:HIS:HD2	1:E:29:ASP:H	1.24	0.83
1:C:545:LEU:O	1:C:550:ALA:HB3	1.78	0.83
2:B:551:ARG:HH11	2:B:551:ARG:HG3	1.43	0.83
1:C:836:GLN:HE21	1:C:836:GLN:H	1.24	0.82
1:A:140:GLU:HG3	1:A:188:ILE:CD1	2.10	0.82
1:E:155:VAL:HG21	1:E:202:VAL:HG21	1.61	0.82
1:E:552:VAL:HG22	1:E:553:PRO:CD	2.10	0.82
2:B:477:LEU:HD22	2:B:551:ARG:HB2	1.61	0.81
1:E:694:HIS:O	1:E:700:ARG:HD3	1.81	0.81
1:A:694:HIS:O	1:A:700:ARG:HD3	1.81	0.81
2:B:455:VAL:C	2:B:456:ARG:HD2	2.01	0.81
1:C:291:PHE:HE1	1:C:315:GLU:HB2	1.46	0.81
1:C:694:HIS:HD2	1:C:696:ASP:H	1.28	0.81
2:B:440:HIS:HB2	2:B:471:ILE:HG22	1.63	0.80
2:D:417:TRP:CE2	2:D:568:PRO:HB2	2.16	0.80
1:E:26:ALA:HB2	1:E:128:VAL:HB	1.61	0.80
1:E:334:LEU:O	1:E:338:ILE:HG12	1.82	0.80
1:C:810:ASP:OD1	1:C:812:THR:HG22	1.81	0.80
1:C:225:PHE:HE2	1:C:277:ILE:HG23	1.45	0.80
2:D:477:LEU:HD13	2:D:551:ARG:NH1	1.96	0.80
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.16	0.80
1:E:237:LYS:HA	1:E:240:MET:HB3	1.63	0.80
1:A:500:ASP:HB2	1:A:552:VAL:HG11	1.63	0.79
1:C:644:ASN:ND2	1:C:684:VAL:H	1.78	0.79
1:E:152:LYS:HD2	1:E:200:VAL:HG23	1.64	0.79
1:C:484:SER:HB3	1:C:797:VAL:HG22	1.63	0.79
1:C:229:TYR:CE2	1:C:276:PHE:HB3	2.18	0.79
1:E:784:LEU:HD23	1:E:794:PRO:HG3	1.63	0.79
2:F:488:ASP:OD2	2:F:492:ARG:HB2	1.82	0.79
1:C:256:LYS:HD3	1:C:257:TRP:N	1.97	0.78
1:A:27:HIS:HD2	1:A:29:ASP:H	1.32	0.78
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.83	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:LYS:HD2	1:E:200:VAL:CG2	2.13	0.78
2:D:527:VAL:HG13	2:D:542:ILE:HD12	1.66	0.77
1:E:490:GLN:HB3	1:E:531:ALA:HB2	1.64	0.77
1:C:229:TYR:CZ	1:C:276:PHE:HB3	2.18	0.77
1:E:404:THR:HG22	1:E:449:PRO:HA	1.66	0.77
1:C:25:ILE:HD12	1:C:125:ALA:HB1	1.66	0.77
1:C:251:ASN:HB2	1:C:254:THR:OG1	1.84	0.77
1:E:694:HIS:CD2	1:E:696:ASP:H	1.99	0.77
1:C:311:GLU:HA	1:C:314:LEU:HD13	1.65	0.77
1:A:140:GLU:HG3	1:A:188:ILE:HD13	1.66	0.77
1:E:147:LEU:CD1	1:E:192:TYR:HB2	2.15	0.77
1:C:552:VAL:HG22	1:C:553:PRO:CD	2.14	0.76
1:E:552:VAL:HG22	1:E:553:PRO:HD2	1.67	0.76
1:E:459:ILE:HG21	1:E:463:LEU:HD12	1.67	0.76
1:C:644:ASN:HD22	1:C:684:VAL:H	1.30	0.76
1:C:225:PHE:CD2	1:C:277:ILE:HG12	2.20	0.76
1:C:578:LYS:HE3	1:C:840:ASP:OD1	1.85	0.76
2:D:531:ILE:HD12	2:D:533:HIS:CE1	2.19	0.76
1:E:71:LYS:HB3	1:E:386:VAL:HG23	1.68	0.76
1:A:819:VAL:O	1:A:823:ARG:HG3	1.85	0.76
1:C:836:GLN:NE2	1:C:836:GLN:H	1.84	0.76
1:A:45:ILE:HD11	1:A:78:TYR:CB	2.16	0.75
1:A:258:THR:HG22	1:A:259:ASN:N	2.00	0.75
1:A:734:GLN:HE21	1:A:734:GLN:N	1.84	0.75
1:C:543:GLN:HG2	1:C:544:ASP:N	2.01	0.75
1:A:561:VAL:HG21	1:A:775:ASN:HA	1.69	0.75
1:A:584:ASN:HD22	1:A:693:LEU:HA	1.50	0.75
1:C:2:VAL:HG22	1:C:3:ALA:H	1.51	0.75
1:C:533:THR:H	1:C:537:HIS:CD2	2.05	0.75
1:A:10:ARG:HD3	1:A:445:ILE:HD11	1.69	0.75
2:B:495:ASN:HD22	2:B:495:ASN:H	1.33	0.75
1:C:315:GLU:CA	1:C:319:LEU:HB2	2.16	0.74
1:A:83:ASP:O	1:A:87:LYS:HD3	1.87	0.74
1:A:321:LYS:O	1:A:325:ARG:HG3	1.87	0.74
1:E:279:ASP:HB3	1:E:280:PRO:HD3	1.69	0.74
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.69	0.74
1:E:391:LYS:HB3	1:E:393:ARG:HG2	1.68	0.74
1:A:429:LYS:HG3	1:A:430:ALA:H	1.52	0.74
1:A:729:PHE:CE2	1:A:774:VAL:HG22	2.23	0.74
1:E:27:HIS:CD2	1:E:29:ASP:H	2.05	0.74
1:E:338:ILE:HG23	1:E:342:LEU:HD12	1.70	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:417:TRP:CE2	2:F:568:PRO:HB2	2.23	0.73
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.18	0.73
2:D:477:LEU:HB2	2:D:551:ARG:HD2	1.70	0.73
1:E:26:ALA:CB	1:E:128:VAL:HB	2.18	0.73
1:A:581:ASN:HB3	1:A:583:HIS:HD2	1.52	0.73
2:F:552:LEU:HD12	2:F:552:LEU:N	2.04	0.73
1:A:406:LYS:HG3	1:A:409:GLN:HB2	1.70	0.73
1:C:258:THR:HG22	1:C:260:LYS:H	1.51	0.73
2:B:405:GLY:HA2	1:C:627:VAL:HG12	1.69	0.73
2:F:487:PRO:HA	2:F:492:ARG:O	1.88	0.73
1:A:459:ILE:HG21	1:A:463:LEU:HD12	1.71	0.73
1:C:515:ASP:HB3	1:C:518:VAL:HG12	1.71	0.73
1:E:288:ILE:HG23	1:E:319:LEU:HD23	1.71	0.73
1:C:536:LEU:HD12	1:C:537:HIS:N	2.04	0.72
1:C:584:ASN:ND2	1:C:694:HIS:H	1.87	0.72
1:A:654:GLN:HG2	1:A:655:TYR:CD2	2.24	0.72
1:C:492:ALA:HA	1:C:528:HIS:O	1.88	0.72
1:C:472:SER:HB3	1:C:475:ALA:HB2	1.72	0.72
2:B:427:ARG:O	2:B:431:GLU:HG3	1.89	0.72
1:C:703:GLY:HA2	2:D:493:ILE:HD13	1.70	0.72
1:A:533:THR:N	1:A:537:HIS:HD2	1.88	0.71
1:A:220:PHE:HB3	1:A:328:LEU:HD13	1.72	0.71
1:A:149:GLU:HA	1:A:355:GLN:HE22	1.55	0.71
1:C:584:ASN:HD21	1:C:694:HIS:H	1.39	0.71
1:C:296:ILE:HD13	1:C:319:LEU:HD21	1.71	0.71
1:E:39:LEU:O	1:E:39:LEU:HD23	1.91	0.71
1:C:509:LYS:HD2	1:C:509:LYS:N	2.03	0.71
1:C:2:VAL:HG22	1:C:3:ALA:N	2.05	0.71
1:C:251:ASN:OD1	1:C:269:LEU:HD11	1.91	0.70
1:E:71:LYS:HE3	1:E:387:PRO:CD	2.19	0.70
1:E:728:VAL:HB	1:E:800:HIS:CD2	2.26	0.70
1:E:694:HIS:HD2	1:E:696:ASP:N	1.88	0.70
1:E:300:LEU:HG	1:E:305:ILE:HB	1.74	0.70
1:E:685:ARG:HE	1:E:687:ASN:HD21	1.39	0.70
1:C:523:SER:OG	1:C:527:GLU:HB2	1.91	0.70
1:C:535:GLU:O	1:C:539:GLU:HG3	1.92	0.70
2:D:531:ILE:HD11	2:D:533:HIS:O	1.91	0.70
2:D:465:ILE:H	2:D:465:ILE:HD13	1.57	0.70
1:C:291:PHE:CE1	1:C:315:GLU:HB2	2.25	0.70
1:E:185:VAL:O	1:E:189:VAL:HG23	1.91	0.70
1:E:578:LYS:HE3	1:E:840:ASP:OD1	1.91	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ILE:HG13	1:A:685:ARG:HE	1.55	0.70
1:C:494:GLU:O	1:C:555:LYS:HB3	1.91	0.70
1:E:10:ARG:HG3	1:E:10:ARG:HH11	1.56	0.70
2:B:551:ARG:NH1	2:B:551:ARG:HG3	2.01	0.69
2:B:495:ASN:ND2	2:B:495:ASN:H	1.89	0.69
1:E:647:ILE:HG13	1:E:685:ARG:HE	1.54	0.69
1:A:338:ILE:HG23	1:A:342:LEU:HD12	1.75	0.69
1:E:757:GLU:HG3	1:E:768:VAL:HG22	1.74	0.69
1:C:545:LEU:O	1:C:550:ALA:CB	2.40	0.69
1:C:220:PHE:HA	1:C:224:GLN:OE1	1.91	0.69
1:C:45:ILE:HD11	1:C:78:TYR:CB	2.23	0.69
1:E:109:VAL:HG21	1:E:138:GLN:HG3	1.73	0.69
1:E:236:ASP:OD1	1:E:238:ALA:HB3	1.91	0.69
1:E:524:GLU:HG3	1:E:669:TRP:CZ3	2.26	0.69
1:A:611:ASP:OD2	1:A:613:LYS:HB2	1.93	0.69
1:E:700:ARG:O	1:E:705:ILE:HD13	1.93	0.69
1:A:36:THR:HG23	1:A:102:LEU:HD21	1.73	0.69
1:C:404:THR:HG22	1:C:449:PRO:CA	2.18	0.69
1:E:321:LYS:O	1:E:325:ARG:HG3	1.92	0.69
1:A:392:GLY:HA2	1:A:513:LYS:HE2	1.74	0.69
1:E:500:ASP:OD2	1:E:552:VAL:HG21	1.92	0.69
1:E:699:DDE:HAA1	3:E:843:APR:H5'2	1.74	0.69
1:C:110:ASP:OD1	1:C:781:THR:HG21	1.93	0.69
2:F:427:ARG:O	2:F:431:GLU:HG3	1.93	0.68
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.76	0.68
1:E:311:GLU:HB3	1:E:322:VAL:HG11	1.75	0.68
1:E:141:THR:HA	1:E:144:ARG:NH2	2.08	0.68
1:E:472:SER:HB3	1:E:475:ALA:HB2	1.75	0.68
1:A:148:GLY:HA2	1:A:760:ARG:NH2	2.08	0.68
1:C:387:PRO:HG3	1:C:394:PHE:CE1	2.29	0.68
1:A:429:LYS:HE3	1:A:430:ALA:H	1.59	0.68
1:E:581:ASN:HD21	1:E:704:GLN:HG3	1.58	0.68
1:E:338:ILE:O	1:E:342:LEU:HB2	1.94	0.68
1:E:581:ASN:O	1:E:582:LYS:HB2	1.94	0.68
1:E:647:ILE:HG13	1:E:685:ARG:NE	2.09	0.68
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.76	0.67
1:A:25:ILE:HD12	1:A:125:ALA:HB1	1.76	0.67
2:F:505:ARG:HH11	2:F:505:ARG:HG3	1.59	0.67
1:C:42:ARG:HG3	1:C:331:ALA:HB3	1.77	0.67
1:E:503:LYS:HB3	1:E:551:GLY:HA3	1.75	0.67
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.75	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:SER:HA	1:C:439:GLY:O	1.95	0.67
1:E:292:LYS:HD3	1:E:295:GLU:OE2	1.95	0.67
1:E:597:VAL:O	1:E:601:ILE:HG13	1.94	0.67
1:A:35:LEU:HD22	1:A:334:LEU:HD11	1.77	0.67
2:B:473:GLY:HA3	2:B:597:LEU:HD11	1.77	0.67
1:C:288:ILE:HG23	1:C:319:LEU:HD23	1.77	0.67
1:A:132:ILE:HD12	1:A:162:ARG:NE	2.09	0.67
1:C:348:ALA:O	1:C:352:ARG:HB2	1.95	0.67
1:C:591:GLU:O	1:C:685:ARG:HB3	1.95	0.67
2:B:524:ALA:O	2:B:528:GLU:HG3	1.95	0.66
1:E:699:DDE:HAA1	3:E:843:APR:C5'	2.26	0.66
1:A:27:HIS:CD2	1:A:29:ASP:H	2.14	0.66
1:C:284:LEU:O	1:C:288:ILE:HB	1.95	0.66
1:E:429:LYS:HG3	1:E:462:PHE:CZ	2.30	0.66
2:D:527:VAL:O	2:D:531:ILE:HG23	1.96	0.66
1:E:707:PRO:O	1:E:711:ARG:HG3	1.95	0.66
1:E:91:GLN:HE22	1:E:344:SER:N	1.91	0.66
1:C:277:ILE:O	1:C:280:PRO:HD2	1.96	0.66
1:C:546:GLU:HG3	1:C:547:HIS:CD2	2.31	0.66
2:B:457:ALA:HB2	2:B:558:TRP:CD2	2.30	0.66
1:C:659:ILE:O	1:C:663:VAL:HG23	1.95	0.66
1:A:348:ALA:HA	1:A:351:TYR:CE2	2.31	0.65
1:A:391:LYS:HG3	1:A:392:GLY:H	1.59	0.65
1:C:454:ILE:HG13	1:C:455:GLY:H	1.61	0.65
1:C:544:ASP:HB3	1:C:549:HIS:CD2	2.32	0.65
1:C:627:VAL:HG21	1:C:631:ARG:NH2	2.10	0.65
1:A:644:ASN:HD22	1:A:684:VAL:H	1.43	0.65
2:D:561:ALA:O	2:D:564:THR:HG23	1.96	0.65
1:E:734:GLN:N	1:E:734:GLN:HE21	1.94	0.65
1:A:594:ASP:HB2	1:A:597:VAL:HG23	1.79	0.65
1:A:784:LEU:HD23	1:A:794:PRO:HG3	1.77	0.65
1:A:627:VAL:CG1	2:F:405:GLY:HA2	2.25	0.65
2:B:546:GLU:HG3	2:B:547:GLU:CG	2.19	0.65
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.78	0.65
1:C:171:LYS:HG2	1:C:282:PHE:CD1	2.32	0.65
2:D:473:GLY:HA3	2:D:597:LEU:HD11	1.79	0.65
1:E:142:VAL:O	1:E:145:GLN:HB2	1.96	0.65
1:E:496:LYS:HD3	1:E:555:LYS:HE2	1.78	0.65
1:C:3:ALA:HA	1:C:46:ILE:O	1.97	0.65
1:E:563:TYR:O	1:E:564:ARG:HD2	1.96	0.65
1:A:493:VAL:CG1	1:A:554:LEU:HD22	2.27	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:THR:H	1:C:537:HIS:HD2	1.45	0.65
1:C:707:PRO:O	1:C:711:ARG:HG3	1.96	0.65
1:C:491:VAL:O	1:C:529:ILE:HA	1.97	0.65
1:A:454:ILE:HG13	1:A:455:GLY:H	1.62	0.64
1:A:465:LYS:HD2	1:A:517:CYS:SG	2.37	0.64
1:A:156:VAL:HG22	1:A:210:ALA:HB3	1.79	0.64
1:C:530:VAL:HG13	1:C:530:VAL:O	1.97	0.64
1:E:219:ALA:HB3	1:E:330:ALA:HA	1.79	0.64
1:E:739:ALA:HB2	1:E:791:GLN:OE1	1.97	0.64
1:A:581:ASN:HB3	1:A:583:HIS:CD2	2.31	0.64
1:E:584:ASN:HD21	1:E:694:HIS:H	1.45	0.64
1:E:379:MET:HB2	1:E:402:ALA:HB3	1.79	0.64
1:E:627:VAL:O	1:E:631:ARG:HG3	1.97	0.64
1:A:132:ILE:HD12	1:A:162:ARG:CD	2.28	0.64
1:C:546:GLU:HB3	1:C:554:LEU:HD12	1.79	0.64
1:E:584:ASN:ND2	1:E:694:HIS:H	1.96	0.64
1:E:749:LYS:HG3	1:E:750:LYS:HD2	1.80	0.64
2:F:503:VAL:HG12	2:F:564:THR:HG22	1.79	0.64
1:C:10:ARG:HD3	1:C:445:ILE:HD11	1.78	0.64
1:E:226:ALA:O	1:E:230:ALA:HB2	1.98	0.64
2:F:524:ALA:O	2:F:528:GLU:HG3	1.97	0.64
1:A:222:ILE:HG22	1:A:241:MET:HB2	1.80	0.63
1:E:432:GLN:HB2	1:E:457:VAL:O	1.97	0.63
1:A:647:ILE:HB	1:A:687:ASN:HD22	1.64	0.63
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.28	0.63
1:A:228:ARG:HH12	1:A:327:PHE:HE1	1.44	0.63
1:A:378:LEU:HD22	1:A:409:GLN:HE22	1.63	0.63
1:C:253:LYS:CA	1:C:253:LYS:HE3	2.24	0.63
1:C:694:HIS:O	1:C:700:ARG:HD3	1.99	0.63
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.80	0.63
1:E:365:ASN:O	1:E:369:ILE:HG12	1.98	0.63
1:C:5:THR:OG1	1:C:8:GLN:HG3	1.99	0.63
1:C:591:GLU:CG	1:C:685:ARG:HG2	2.28	0.63
2:D:432:ARG:HA	2:D:432:ARG:CZ	2.29	0.63
2:F:530:LEU:HA	2:F:604:PRO:HG3	1.81	0.63
1:A:156:VAL:HG21	1:A:334:LEU:CD2	2.29	0.63
1:E:493:VAL:HA	1:E:556:ILE:CD1	2.29	0.63
1:E:454:ILE:HG13	1:E:455:GLY:N	2.14	0.62
1:A:581:ASN:O	1:A:582:LYS:HB2	1.97	0.62
1:C:730:LEU:HB2	1:C:799:ASP:HB2	1.81	0.62
1:A:19:VAL:O	1:A:345:PRO:HD3	2.00	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HG3	1:A:430:ALA:N	2.13	0.62
1:C:484:SER:HB3	1:C:797:VAL:CG2	2.28	0.62
2:D:450:ILE:O	2:D:454:GLY:HA2	2.00	0.62
1:E:126:LEU:HD11	1:E:156:VAL:HG21	1.81	0.62
1:E:391:LYS:HG3	1:E:392:GLY:H	1.65	0.62
1:A:410:LYS:HA	1:A:430:ALA:HA	1.81	0.62
1:C:494:GLU:HG2	1:C:528:HIS:CE1	2.34	0.62
1:E:331:ALA:O	1:E:335:LEU:HG	1.99	0.62
1:A:710:ARG:NH1	1:A:710:ARG:HG3	2.09	0.62
1:C:384:LYS:HB2	1:C:465:LYS:NZ	2.15	0.62
1:C:584:ASN:HD22	1:C:693:LEU:HA	1.64	0.62
1:E:126:LEU:HD11	1:E:156:VAL:CG2	2.30	0.62
1:E:45:ILE:HD11	1:E:78:TYR:HB3	1.80	0.62
2:F:517:THR:HG21	2:F:548:GLU:HA	1.81	0.62
1:A:466:THR:HG22	1:A:467:GLY:N	2.14	0.62
1:A:536:LEU:O	1:A:540:ILE:HG12	2.00	0.62
1:E:158:ASN:ND2	1:E:159:LYS:HG3	2.15	0.62
2:F:470:TYR:CE2	2:F:555:ILE:HG12	2.35	0.62
1:E:78:TYR:HE1	1:E:97:SER:HB3	1.64	0.62
1:E:74:ALA:O	1:E:439:GLY:HA2	2.00	0.61
1:A:493:VAL:HG12	1:A:554:LEU:HD22	1.83	0.61
2:B:467:ARG:HG3	2:B:558:TRP:CD1	2.36	0.61
1:C:703:GLY:HA2	2:D:493:ILE:CD1	2.30	0.61
1:E:552:VAL:HG22	1:E:553:PRO:HD3	1.81	0.61
1:E:836:GLN:HE21	1:E:836:GLN:H	1.49	0.61
1:A:19:VAL:HG22	1:A:99:LEU:HB3	1.81	0.61
1:C:522:MET:HA	1:C:527:GLU:O	1.99	0.61
1:E:39:LEU:HD21	1:E:77:LEU:CD2	2.31	0.61
1:C:239:LYS:O	1:C:243:ARG:HG3	2.01	0.61
1:C:591:GLU:HG2	1:C:685:ARG:HG2	1.81	0.61
2:D:457:ALA:HB2	2:D:558:TRP:CD2	2.36	0.61
1:A:140:GLU:HG3	1:A:188:ILE:HD11	1.82	0.61
1:A:731:VAL:HG12	1:A:796:MET:CB	2.30	0.61
1:E:91:GLN:NE2	1:E:344:SER:H	1.91	0.61
1:E:381:TYR:O	1:E:398:GLY:HA3	1.99	0.61
1:C:70:ILE:O	1:C:440:ARG:HG3	2.01	0.61
1:E:464:LEU:HD21	1:E:485:VAL:HB	1.82	0.61
1:C:414:GLN:HB3	1:C:418:TYR:CD2	2.36	0.60
1:C:669:TRP:HD1	1:C:710:ARG:HE	1.44	0.60
1:E:39:LEU:CD2	1:E:77:LEU:HG	2.31	0.60
1:A:454:ILE:HG13	1:A:455:GLY:N	2.14	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:MET:O	1:A:13:MET:HG3	2.02	0.60
1:C:189:VAL:CG1	1:C:200:VAL:HG12	2.31	0.60
1:C:76:SER:O	1:C:77:LEU:HD12	2.01	0.60
1:E:279:ASP:O	1:E:283:ARG:HG2	2.02	0.60
1:A:464:LEU:HD21	1:A:485:VAL:HB	1.83	0.60
2:B:490:ARG:HH22	2:B:492:ARG:NE	1.99	0.60
1:A:229:TYR:CE2	1:A:276:PHE:HB3	2.36	0.60
1:E:240:MET:O	1:E:244:LEU:HG	2.00	0.60
2:B:417:TRP:CE2	2:B:568:PRO:HB2	2.36	0.60
1:C:348:ALA:HA	1:C:351:TYR:CE2	2.36	0.60
1:C:89:ILE:HG22	1:C:91:GLN:HG2	1.84	0.60
1:E:501:LEU:HB3	1:E:502:PRO:HD3	1.82	0.60
1:E:730:LEU:HB2	1:E:799:ASP:HB2	1.83	0.60
1:A:823:ARG:NH1	1:A:829:LYS:O	2.35	0.60
2:B:488:ASP:OD2	2:B:492:ARG:HD2	2.01	0.60
1:E:132:ILE:N	1:E:132:ILE:HD12	2.17	0.60
1:A:2:VAL:HG22	1:A:3:ALA:N	2.16	0.60
1:A:581:ASN:HD21	1:A:704:GLN:HG3	1.66	0.60
1:C:386:VAL:HG11	1:C:437:MET:CE	2.32	0.60
1:E:281:ILE:HG12	1:E:327:PHE:HE2	1.67	0.60
1:E:75:ILE:HD13	1:E:439:GLY:CA	2.31	0.60
1:C:406:LYS:HB3	1:C:447:ASP:HB3	1.82	0.60
2:F:484:ASP:OD2	2:F:494:ARG:HG2	2.02	0.60
1:E:43:ALA:HB1	1:E:78:TYR:O	2.02	0.60
1:A:103:ILE:HD11	1:A:453:ILE:HG12	1.84	0.59
1:C:354:GLU:OE2	1:C:361:ALA:HB1	2.02	0.59
1:C:529:ILE:N	1:C:529:ILE:HD12	2.17	0.59
1:E:10:ARG:HG3	1:E:10:ARG:NH1	2.17	0.59
2:B:551:ARG:CG	2:B:551:ARG:HH11	2.15	0.59
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.84	0.59
1:E:546:GLU:HB2	1:E:554:LEU:HD12	1.83	0.59
1:C:285:PHE:HE2	1:C:324:MET:SD	2.25	0.59
1:C:581:ASN:O	1:C:582:LYS:HB2	2.01	0.59
1:E:186:ASN:CG	1:E:201:GLN:HE21	2.06	0.59
1:E:348:ALA:HA	1:E:351:TYR:CE2	2.37	0.59
1:C:132:ILE:HG23	1:C:133:GLU:N	2.18	0.59
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.37	0.59
1:C:669:TRP:HE1	1:C:710:ARG:NH2	2.01	0.59
1:A:520:THR:HA	1:A:529:ILE:O	2.02	0.59
1:C:150:ARG:HD3	1:C:197:LEU:HD21	1.85	0.59
1:A:220:PHE:HA	1:A:224:GLN:OE1	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ILE:HB	1:A:687:ASN:ND2	2.18	0.59
1:A:737:GLU:HG3	1:A:766:PHE:CD2	2.38	0.59
1:C:231:LYS:HE3	1:C:232:LYS:CG	2.28	0.59
1:E:39:LEU:HG	1:E:335:LEU:HD21	1.84	0.59
2:F:457:ALA:HB2	2:F:558:TRP:CD2	2.38	0.59
1:A:30:HIS:HA	1:A:159:LYS:HE3	1.85	0.58
1:C:606:ILE:HD12	1:C:619:MET:HG2	1.84	0.58
1:E:395:TYR:CE1	1:E:457:VAL:HG13	2.38	0.58
2:F:493:ILE:HG22	2:F:493:ILE:O	2.03	0.58
1:A:758:GLU:HG3	1:A:767:THR:HG23	1.86	0.58
1:E:647:ILE:HB	1:E:687:ASN:HD22	1.67	0.58
1:E:685:ARG:NE	1:E:687:ASN:HD21	2.01	0.58
1:A:26:ALA:HB2	1:A:128:VAL:HB	1.85	0.58
1:C:155:VAL:HG21	1:C:185:VAL:HG11	1.85	0.58
1:C:594:ASP:HB2	1:C:597:VAL:HG23	1.86	0.58
1:E:26:ALA:O	1:E:32:LYS:HD2	2.03	0.58
1:E:348:ALA:O	1:E:352:ARG:HB2	2.03	0.58
1:E:737:GLU:HG3	1:E:766:PHE:CE1	2.38	0.58
1:A:690:ASP:OD1	1:A:691:VAL:N	2.35	0.58
1:A:698:ILE:HD13	1:A:698:ILE:N	2.18	0.58
1:C:256:LYS:HA	1:C:256:LYS:HE2	1.85	0.58
1:C:268:PRO:O	1:C:269:LEU:HD23	2.04	0.58
1:C:225:PHE:HD2	1:C:277:ILE:HG12	1.67	0.58
1:C:490:GLN:HB2	1:C:529:ILE:CG2	2.33	0.58
1:E:181:THR:O	1:E:185:VAL:HG23	2.04	0.58
2:B:457:ALA:HB2	2:B:558:TRP:CE3	2.38	0.58
1:E:155:VAL:CG2	1:E:202:VAL:HG21	2.32	0.58
1:A:647:ILE:HG13	1:A:685:ARG:NE	2.17	0.58
1:A:584:ASN:ND2	1:A:694:HIS:H	2.01	0.58
1:A:584:ASN:HD21	1:A:694:HIS:H	1.51	0.58
1:A:3:ALA:HA	1:A:46:ILE:O	2.04	0.58
1:A:321:LYS:NZ	1:A:325:ARG:HD3	2.19	0.58
1:E:411:VAL:HG12	1:E:412:ARG:N	2.18	0.58
1:E:68:ILE:HG23	1:E:390:ASP:HB2	1.86	0.58
1:E:731:VAL:HG23	1:E:796:MET:HB3	1.84	0.58
1:E:89:ILE:C	1:E:91:GLN:H	2.07	0.58
1:A:591:GLU:CG	1:A:685:ARG:HG2	2.34	0.58
2:B:460:GLN:HB3	2:B:467:ARG:HD3	1.86	0.58
1:E:581:ASN:HB3	1:E:583:HIS:HD2	1.69	0.58
1:E:307:LEU:HD13	1:E:312:LYS:HA	1.86	0.57
2:F:508:LEU:N	2:F:509:PRO:CD	2.67	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLN:HE21	1:A:411:VAL:CG2	2.15	0.57
1:A:411:VAL:HG12	1:A:412:ARG:N	2.19	0.57
1:A:644:ASN:ND2	1:A:684:VAL:H	2.01	0.57
1:A:836:GLN:HE21	1:A:836:GLN:H	1.52	0.57
1:C:597:VAL:O	1:C:601:ILE:HG13	2.03	0.57
1:E:69:THR:OG1	1:E:389:SER:HB3	2.03	0.57
1:E:132:ILE:HD13	1:E:162:ARG:HD3	1.87	0.57
1:E:387:PRO:HG3	1:E:394:PHE:CE1	2.40	0.57
1:A:578:LYS:HE3	1:A:840:ASP:OD1	2.05	0.57
1:C:221:THR:OG1	1:C:224:GLN:HG3	2.05	0.57
1:C:211:PHE:O	1:C:219:ALA:HA	2.05	0.57
1:C:243:ARG:NH1	1:C:257:TRP:CD1	2.73	0.57
1:E:103:ILE:HD12	1:E:103:ILE:N	2.18	0.57
1:E:183:GLU:O	1:E:187:VAL:HG23	2.04	0.57
2:F:422:LEU:HD13	2:F:594:ILE:HD11	1.87	0.57
1:C:288:ILE:HG23	1:C:319:LEU:CD2	2.34	0.57
1:C:799:ASP:OD1	1:C:800:HIS:HD2	1.88	0.57
2:D:479:TYR:CD2	2:D:582:LEU:HB2	2.40	0.57
2:D:484:ASP:OD2	2:D:494:ARG:HG2	2.04	0.57
1:E:284:LEU:HD13	1:E:324:MET:CE	2.35	0.57
1:E:536:LEU:O	1:E:539:GLU:N	2.38	0.57
1:A:235:VAL:HG21	1:A:240:MET:HB2	1.87	0.57
1:A:501:LEU:C	1:A:501:LEU:HD23	2.25	0.57
2:D:457:ALA:HB2	2:D:558:TRP:CE3	2.40	0.57
1:E:581:ASN:ND2	1:E:704:GLN:HG3	2.19	0.57
1:E:589:LYS:HE3	1:E:689:LEU:HD11	1.86	0.57
1:A:106:PRO:HG3	1:A:114:GLU:HG3	1.87	0.57
1:A:836:GLN:NE2	1:A:836:GLN:H	2.02	0.57
1:C:35:LEU:HD22	1:C:334:LEU:HD11	1.85	0.57
1:E:229:TYR:CD1	1:E:232:LYS:HD2	2.40	0.57
1:E:611:ASP:OD2	1:E:613:LYS:HB2	2.05	0.57
1:C:569:SER:O	1:C:720:ALA:HB1	2.05	0.56
1:E:36:THR:O	1:E:40:VAL:HG23	2.06	0.56
1:C:273:PHE:CD1	1:C:277:ILE:HD12	2.40	0.56
1:C:311:GLU:HA	1:C:314:LEU:CD1	2.33	0.56
1:E:81:MET:O	1:E:96:ASN:HB3	2.05	0.56
2:D:546:GLU:CG	2:D:547:GLU:HG3	2.19	0.56
1:E:736:PRO:HB2	1:E:738:GLN:HG2	1.87	0.56
1:A:155:VAL:HG12	1:A:156:VAL:N	2.19	0.56
1:A:226:ALA:CB	1:A:241:MET:HB3	2.34	0.56
1:C:200:VAL:O	1:C:200:VAL:CG1	2.53	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ALA:CB	1:C:241:MET:HB3	2.35	0.56
1:E:496:LYS:HD3	1:E:555:LYS:CE	2.35	0.56
1:A:251:ASN:HB3	1:A:254:THR:OG1	2.05	0.56
1:C:565:GLU:O	1:C:681:MET:HA	2.06	0.56
2:D:492:ARG:HH12	2:D:494:ARG:HD2	1.70	0.56
1:C:390:ASP:O	1:C:391:LYS:HB2	2.05	0.56
1:E:503:LYS:HB3	1:E:551:GLY:CA	2.36	0.56
2:F:505:ARG:NH1	2:F:505:ARG:HG3	2.20	0.56
1:A:365:ASN:O	1:A:369:ILE:HG12	2.06	0.56
1:E:285:PHE:CE2	1:E:320:LEU:HD11	2.41	0.56
1:E:565:GLU:O	1:E:681:MET:HA	2.05	0.56
1:A:258:THR:CG2	1:A:259:ASN:H	2.16	0.56
2:B:488:ASP:OD1	2:B:489:ALA:N	2.39	0.56
1:E:555:LYS:O	1:E:556:ILE:HD13	2.05	0.56
1:A:381:TYR:O	1:A:398:GLY:HA3	2.05	0.56
2:B:563:ARG:HG3	2:B:563:ARG:HH11	1.71	0.56
1:E:152:LYS:CD	1:E:200:VAL:HG23	2.36	0.56
1:E:258:THR:HG22	1:E:259:ASN:N	2.21	0.56
1:E:694:HIS:CE1	1:E:699:DDE:HD2	2.40	0.56
1:A:478:MET:O	1:A:479:LYS:C	2.44	0.56
1:A:820:LEU:HD11	1:A:824:LYS:HE3	1.88	0.56
1:C:240:MET:O	1:C:244:LEU:HG	2.06	0.56
1:A:153:PRO:HD2	1:A:200:VAL:HG13	1.87	0.56
1:C:669:TRP:HE1	1:C:710:ARG:HH21	1.52	0.56
1:E:307:LEU:HD12	1:E:312:LYS:HD3	1.88	0.56
2:F:465:ILE:HD12	2:F:535:LEU:HD12	1.87	0.56
1:C:694:HIS:CD2	1:C:696:ASP:H	2.17	0.55
1:E:810:ASP:O	1:E:816:GLY:HA3	2.07	0.55
1:A:698:ILE:H	1:A:698:ILE:HD13	1.71	0.55
1:C:9:MET:O	1:C:13:MET:HG3	2.05	0.55
1:C:45:ILE:HD11	1:C:78:TYR:HB2	1.89	0.55
1:C:490:GLN:O	1:C:491:VAL:HG13	2.06	0.55
1:C:192:TYR:HA	1:C:763:THR:CG2	2.36	0.55
1:E:561:VAL:HG21	1:E:775:ASN:CB	2.36	0.55
1:C:231:LYS:HG2	1:C:232:LYS:N	2.20	0.55
1:C:733:ILE:HG21	1:C:743:ILE:CD1	2.36	0.55
1:C:735:CYS:SG	1:C:739:ALA:HB3	2.47	0.55
1:E:278:LEU:O	1:E:282:PHE:HB2	2.06	0.55
2:F:433:GLY:O	2:F:505:ARG:HB2	2.07	0.55
1:A:581:ASN:ND2	1:A:704:GLN:HG3	2.22	0.55
1:C:529:ILE:HG22	1:C:530:VAL:N	2.21	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ARG:O	1:E:166:GLU:HB2	2.07	0.55
1:A:707:PRO:O	1:A:711:ARG:HG3	2.06	0.55
1:E:258:THR:HG22	1:E:259:ASN:H	1.71	0.55
1:A:258:THR:CG2	1:A:260:LYS:HG2	2.37	0.55
1:A:763:THR:HB	1:A:764:PRO:HD2	1.87	0.55
2:D:570:ALA:HB3	2:D:591:GLU:OE1	2.07	0.55
1:E:75:ILE:HD13	1:E:439:GLY:HA3	1.89	0.55
1:E:581:ASN:O	1:E:582:LYS:CB	2.55	0.55
1:A:429:LYS:CG	1:A:430:ALA:H	2.19	0.55
1:C:538:LEU:O	1:C:542:LEU:HG	2.06	0.55
1:E:536:LEU:HD11	1:E:540:ILE:HD11	1.88	0.55
1:E:644:ASN:ND2	1:E:684:VAL:H	2.04	0.55
1:E:9:MET:O	1:E:12:LEU:HB3	2.07	0.55
1:E:478:MET:O	1:E:479:LYS:C	2.46	0.55
1:E:495:VAL:HG12	1:E:554:LEU:HD23	1.89	0.55
1:C:544:ASP:O	1:C:549:HIS:N	2.40	0.54
2:D:551:ARG:HG3	2:D:551:ARG:HH11	1.72	0.54
1:E:17:THR:HB	1:E:92:LYS:O	2.07	0.54
1:A:585:ARG:HB2	1:A:692:THR:OG1	2.07	0.54
2:F:400:PHE:CD1	2:F:429:LEU:HD23	2.42	0.54
1:A:485:VAL:O	1:A:487:PRO:HD3	2.07	0.54
2:B:508:LEU:N	2:B:509:PRO:CD	2.69	0.54
1:C:251:ASN:H	1:C:251:ASN:HD22	1.54	0.54
1:C:675:PRO:HD3	1:C:714:TYR:CE1	2.42	0.54
2:D:529:ARG:NH1	2:D:604:PRO:HG2	2.22	0.54
2:F:529:ARG:NH1	2:F:604:PRO:HG2	2.22	0.54
1:A:348:ALA:HA	1:A:351:TYR:CZ	2.43	0.54
1:A:591:GLU:HG2	1:A:685:ARG:HG2	1.90	0.54
1:A:797:VAL:HG22	1:A:798:PHE:N	2.23	0.54
1:C:576:LEU:HD12	1:C:577:SER:N	2.22	0.54
1:E:237:LYS:HA	1:E:240:MET:CB	2.35	0.54
1:E:360:PRO:HB2	1:E:363:ASP:HB2	1.90	0.54
2:F:429:LEU:O	2:F:434:TYR:HB2	2.07	0.54
1:A:81:MET:O	1:A:96:ASN:HB3	2.08	0.54
1:C:106:PRO:HG3	1:C:114:GLU:HG3	1.88	0.54
1:E:303:LEU:O	1:E:304:GLU:HB2	2.08	0.54
1:E:569:SER:O	1:E:720:ALA:HB1	2.07	0.54
1:A:784:LEU:CD2	1:A:794:PRO:HG3	2.37	0.54
1:C:581:ASN:ND2	1:C:699:DDE:O	2.40	0.54
1:C:627:VAL:O	1:C:631:ARG:HG3	2.08	0.54
1:C:650:THR:CG2	1:C:688:ILE:HG22	2.38	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:171:LYS:NZ	1:E:283:ARG:NH2	2.56	0.54
1:A:111:PHE:HB3	1:A:114:GLU:HG2	1.90	0.54
1:A:729:PHE:CD2	1:A:774:VAL:HG22	2.43	0.54
1:A:669:TRP:CZ2	2:B:490:ARG:NH1	2.76	0.54
1:E:495:VAL:HA	1:E:554:LEU:HA	1.90	0.54
2:B:410:SER:HB3	2:B:413:GLY:O	2.07	0.54
1:C:132:ILE:HG23	1:C:133:GLU:H	1.73	0.54
1:C:320:LEU:HD12	1:C:324:MET:HG3	1.90	0.54
1:C:750:LYS:O	1:C:751:ARG:HB2	2.07	0.54
2:D:505:ARG:HG3	2:D:505:ARG:HH11	1.73	0.54
2:F:420:GLU:H	2:F:420:GLU:CD	2.12	0.54
1:A:589:LYS:HE3	1:A:689:LEU:HD11	1.90	0.54
1:C:291:PHE:HE1	1:C:315:GLU:CB	2.20	0.54
2:F:535:LEU:HB3	2:F:536:PRO:HA	1.89	0.54
1:A:307:LEU:HD13	1:A:312:LYS:HA	1.90	0.53
1:A:727:PRO:HG2	1:A:774:VAL:HB	1.88	0.53
1:C:26:ALA:HB2	1:C:128:VAL:HB	1.88	0.53
2:F:531:ILE:HG22	2:F:533:HIS:H	1.72	0.53
1:C:155:VAL:HG12	1:C:156:VAL:N	2.21	0.53
1:E:186:ASN:HB2	1:E:201:GLN:HG2	1.90	0.53
2:F:440:HIS:HB2	2:F:471:ILE:HG22	1.90	0.53
1:A:45:ILE:CD1	1:A:78:TYR:HB2	2.29	0.53
1:C:234:GLY:O	1:C:235:VAL:HG23	2.08	0.53
1:C:614:ALA:O	1:C:618:ILE:HG12	2.07	0.53
1:A:258:THR:HG22	1:A:260:LYS:H	1.73	0.53
1:A:694:HIS:CD2	1:A:696:ASP:H	2.07	0.53
1:C:331:ALA:O	1:C:335:LEU:HG	2.09	0.53
1:C:36:THR:O	1:C:40:VAL:HG23	2.09	0.53
2:D:427:ARG:O	2:D:431:GLU:HG3	2.09	0.53
1:E:108:HIS:O	1:E:111:PHE:HD2	1.90	0.53
1:A:155:VAL:CG1	1:A:156:VAL:N	2.72	0.53
1:A:395:TYR:CE1	1:A:457:VAL:HG13	2.44	0.53
1:C:501:LEU:C	1:C:501:LEU:HD23	2.29	0.53
1:C:606:ILE:HD12	1:C:619:MET:CG	2.39	0.53
1:E:235:VAL:HG11	1:E:239:LYS:HD3	1.91	0.53
1:E:385:MET:HG2	1:E:465:LYS:HA	1.91	0.53
2:F:456:ARG:HH21	2:F:458:ARG:HH21	1.57	0.53
1:A:588:LEU:HD12	1:A:588:LEU:C	2.29	0.53
1:C:591:GLU:HG2	1:C:685:ARG:CG	2.39	0.53
1:E:650:THR:CG2	1:E:688:ILE:HG22	2.38	0.53
1:E:39:LEU:HD21	1:E:77:LEU:HG	1.90	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:823:ARG:NH1	1:E:828:MET:HB2	2.22	0.53
2:D:477:LEU:O	2:D:477:LEU:HD12	2.08	0.53
1:E:167:LEU:H	1:E:167:LEU:HD12	1.73	0.53
2:F:427:ARG:HG2	2:F:428:GLN:N	2.24	0.53
1:C:576:LEU:HD12	1:C:577:SER:H	1.73	0.53
1:A:156:VAL:HG21	1:A:334:LEU:HD22	1.90	0.53
1:E:109:VAL:O	1:E:109:VAL:HG12	2.08	0.53
1:E:759:GLN:HB2	1:E:766:PHE:CE2	2.44	0.53
1:A:186:ASN:HB3	1:A:201:GLN:HE21	1.74	0.52
1:E:644:ASN:HD22	1:E:684:VAL:H	1.57	0.52
2:D:486:GLU:HG3	2:D:487:PRO:HD2	1.91	0.52
1:E:337:MET:HA	1:E:341:HIS:CD2	2.45	0.52
1:E:465:LYS:HD2	1:E:517:CYS:SG	2.49	0.52
1:A:550:ALA:O	1:A:552:VAL:HG23	2.09	0.52
2:D:542:ILE:HG12	2:D:543:THR:N	2.24	0.52
1:E:80:GLU:HA	1:E:96:ASN:O	2.09	0.52
1:C:291:PHE:O	1:C:293:LYS:N	2.43	0.52
1:E:203:TYR:HD2	1:E:206:ARG:HD2	1.73	0.52
2:F:548:GLU:HG2	2:F:548:GLU:O	2.10	0.52
2:F:552:LEU:H	2:F:552:LEU:HD12	1.72	0.52
1:C:314:LEU:HD21	1:C:322:VAL:HG21	1.91	0.52
1:C:386:VAL:HG11	1:C:437:MET:HE1	1.92	0.52
2:D:508:LEU:N	2:D:509:PRO:CD	2.72	0.52
1:A:698:ILE:CD1	1:A:698:ILE:H	2.23	0.52
1:A:4:PHE:HA	1:A:8:GLN:OE1	2.10	0.52
1:C:236:ASP:OD2	1:C:239:LYS:HE2	2.10	0.52
1:C:243:ARG:NH1	1:C:257:TRP:CG	2.78	0.52
1:E:37:ASP:O	1:E:41:GLN:HG3	2.09	0.52
1:E:545:LEU:HD12	1:E:549:HIS:CB	2.35	0.52
1:E:750:LYS:O	1:E:751:ARG:HB2	2.10	0.52
1:A:277:ILE:O	1:A:280:PRO:HD2	2.09	0.52
1:A:486:SER:O	1:A:488:VAL:HG13	2.09	0.52
1:C:515:ASP:HB3	1:C:518:VAL:CG1	2.37	0.52
1:E:411:VAL:HG11	1:E:469:LEU:HB3	1.92	0.52
1:A:411:VAL:HG13	1:A:470:THR:O	2.10	0.52
1:E:337:MET:HA	1:E:341:HIS:HD2	1.75	0.52
1:A:677:PHE:CZ	1:A:679:GLU:HG3	2.45	0.52
1:E:109:VAL:CG2	1:E:138:GLN:HG3	2.39	0.52
1:E:584:ASN:HD22	1:E:693:LEU:HA	1.75	0.52
1:A:186:ASN:HB3	1:A:201:GLN:HG2	1.90	0.51
1:A:112:SER:CB	1:A:794:PRO:O	2.58	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LYS:HG2	1:C:282:PHE:CE1	2.45	0.51
1:C:226:ALA:O	1:C:230:ALA:HB2	2.10	0.51
1:C:588:LEU:C	1:C:588:LEU:HD12	2.31	0.51
1:C:91:GLN:O	1:C:93:THR:HG23	2.11	0.51
1:C:85:ASP:OD1	1:C:223:ARG:NH2	2.43	0.51
1:A:545:LEU:HD12	1:A:549:HIS:HB2	1.92	0.51
1:A:685:ARG:HE	1:A:687:ASN:HD21	1.58	0.51
1:C:158:ASN:ND2	1:C:159:LYS:HG2	2.25	0.51
1:C:25:ILE:CD1	1:C:125:ALA:HB1	2.36	0.51
1:C:500:ASP:OD2	1:C:552:VAL:HG21	2.11	0.51
1:E:739:ALA:HB1	1:E:788:THR:HB	1.93	0.51
2:B:477:LEU:HD13	2:B:551:ARG:NH1	2.25	0.51
1:C:147:LEU:HD11	1:C:189:VAL:HA	1.92	0.51
1:C:164:LEU:HD21	1:C:174:LEU:HD22	1.93	0.51
1:E:176:GLN:O	1:E:180:ARG:HG3	2.10	0.51
1:E:773:PRO:HB2	1:E:776:GLU:HB2	1.91	0.51
2:B:471:ILE:HG21	2:B:501:VAL:HG21	1.91	0.51
1:C:132:ILE:HG23	1:C:133:GLU:HG3	1.91	0.51
1:C:581:ASN:O	1:C:582:LYS:CB	2.58	0.51
1:E:212:GLY:HA3	1:E:219:ALA:HA	1.93	0.51
1:E:350:ALA:O	1:E:370:LYS:HG2	2.11	0.51
2:F:426:HIS:O	2:F:429:LEU:HB2	2.11	0.51
1:E:78:TYR:CE1	1:E:97:SER:HB3	2.46	0.51
1:E:145:GLN:NE2	1:E:793:PHE:CZ	2.78	0.51
1:A:132:ILE:HD12	1:A:162:ARG:CZ	2.41	0.51
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.46	0.51
1:C:155:VAL:CG1	1:C:156:VAL:N	2.73	0.51
1:C:223:ARG:HH11	1:C:223:ARG:HG2	1.74	0.51
1:C:237:LYS:HA	1:C:240:MET:HB3	1.93	0.51
1:E:704:GLN:O	1:E:707:PRO:HD2	2.11	0.51
1:A:306:VAL:HG13	1:A:306:VAL:O	2.11	0.51
1:A:459:ILE:HD11	1:A:469:LEU:HD21	1.93	0.51
1:C:675:PRO:HD3	1:C:714:TYR:CD1	2.46	0.51
1:E:307:LEU:HB2	1:E:312:LYS:HE2	1.93	0.51
1:E:5:THR:OG1	1:E:8:GLN:HG3	2.11	0.51
2:F:504:PRO:HD3	2:F:563:ARG:O	2.11	0.51
2:F:542:ILE:HD12	2:F:543:THR:H	1.76	0.51
1:A:19:VAL:HA	1:A:99:LEU:O	2.11	0.50
2:B:445:GLU:OE1	2:B:494:ARG:NH2	2.40	0.50
1:C:258:THR:HG22	1:C:259:ASN:N	2.25	0.50
1:C:563:TYR:O	1:C:564:ARG:HD2	2.11	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:O	1:A:187:VAL:HG23	2.12	0.50
1:A:89:ILE:HG22	1:A:91:GLN:HG2	1.92	0.50
1:C:129:VAL:HG13	1:C:134:GLY:O	2.10	0.50
1:C:357:TYR:CD2	1:C:366:CYS:HB2	2.46	0.50
1:C:601:ILE:HG12	1:C:606:ILE:HB	1.92	0.50
1:E:371:ASN:O	1:E:372:CYS:C	2.48	0.50
2:D:531:ILE:CD1	2:D:533:HIS:CE1	2.90	0.50
1:E:75:ILE:HD13	1:E:439:GLY:HA2	1.93	0.50
1:E:454:ILE:HG13	1:E:455:GLY:H	1.75	0.50
1:E:607:ASN:HB3	1:E:610:ASP:OD2	2.10	0.50
2:F:473:GLY:HA3	2:F:597:LEU:HD11	1.93	0.50
1:C:306:VAL:HG23	1:C:306:VAL:O	2.11	0.50
2:D:445:GLU:OE1	2:D:494:ARG:NH2	2.44	0.50
1:E:669:TRP:CZ2	2:F:492:ARG:HG2	2.46	0.50
1:E:786:GLN:N	1:E:786:GLN:OE1	2.45	0.50
1:A:501:LEU:HB3	1:A:502:PRO:HD3	1.92	0.50
1:C:27:HIS:CD2	1:C:29:ASP:H	2.15	0.50
1:C:410:LYS:HA	1:C:430:ALA:HA	1.93	0.50
1:C:644:ASN:HD22	1:C:684:VAL:N	2.03	0.50
1:E:186:ASN:OD1	1:E:186:ASN:C	2.50	0.50
1:E:186:ASN:HA	1:E:189:VAL:HB	1.93	0.50
1:E:150:ARG:NH1	1:E:351:TYR:O	2.44	0.50
1:A:288:ILE:HG23	1:A:319:LEU:HD23	1.93	0.50
1:C:192:TYR:HA	1:C:763:THR:HG22	1.94	0.50
1:C:494:GLU:HG2	1:C:528:HIS:HE1	1.74	0.50
1:E:129:VAL:HG12	1:E:130:ASP:N	2.27	0.50
1:E:284:LEU:HD13	1:E:324:MET:HE3	1.93	0.50
1:E:71:LYS:HB3	1:E:386:VAL:CG2	2.38	0.50
2:B:479:TYR:CD2	2:B:582:LEU:HB2	2.46	0.50
2:B:542:ILE:HD12	2:B:543:THR:H	1.76	0.50
1:C:478:MET:O	1:C:479:LYS:C	2.49	0.50
1:C:667:PHE:O	1:C:671:THR:HG23	2.12	0.50
1:C:743:ILE:HD13	1:C:784:LEU:HD11	1.94	0.50
2:D:523:ALA:O	2:D:524:ALA:C	2.50	0.50
1:E:482:LYS:HD3	1:E:797:VAL:HG11	1.92	0.50
1:C:45:ILE:HD11	1:C:78:TYR:HB3	1.94	0.50
1:C:697:ALA:HA	1:C:700:ARG:NE	2.26	0.50
1:E:144:ARG:HG2	1:E:192:TYR:CD2	2.46	0.50
1:E:348:ALA:HA	1:E:351:TYR:CZ	2.47	0.50
1:E:412:ARG:HG2	1:E:412:ARG:HH11	1.76	0.50
1:A:26:ALA:CB	1:A:128:VAL:HB	2.40	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HE3	1:A:430:ALA:N	2.25	0.50
1:C:288:ILE:HG23	1:C:319:LEU:CG	2.42	0.50
1:E:262:THR:CG2	1:E:266:GLY:HA2	2.42	0.50
1:A:200:VAL:O	1:A:200:VAL:HG13	2.10	0.49
1:A:704:GLN:O	1:A:707:PRO:HD2	2.12	0.49
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.94	0.49
1:A:357:TYR:CE2	1:A:359:GLY:HA3	2.47	0.49
1:A:429:LYS:CE	1:A:430:ALA:H	2.25	0.49
1:A:43:ALA:HB1	1:A:78:TYR:O	2.12	0.49
2:B:435:VAL:HG21	2:B:598:PRO:HG3	1.94	0.49
1:C:292:LYS:HD2	1:C:295:GLU:OE2	2.12	0.49
1:E:229:TYR:HD1	1:E:232:LYS:HD2	1.76	0.49
1:E:588:LEU:HD12	1:E:588:LEU:C	2.32	0.49
1:E:836:GLN:NE2	1:E:836:GLN:H	2.09	0.49
2:F:513:ARG:HB2	2:F:513:ARG:NH1	2.15	0.49
1:C:381:TYR:O	1:C:398:GLY:HA3	2.13	0.49
1:E:200:VAL:O	1:E:200:VAL:HG22	2.13	0.49
1:E:496:LYS:HD3	1:E:555:LYS:NZ	2.26	0.49
1:A:561:VAL:HG21	1:A:775:ASN:CA	2.41	0.49
2:B:490:ARG:HH22	2:B:492:ARG:CZ	2.24	0.49
1:C:191:THR:O	1:C:763:THR:HG22	2.12	0.49
2:F:519:ALA:O	2:F:521:PRO:HD3	2.12	0.49
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.77	0.49
1:C:43:ALA:HB1	1:C:78:TYR:O	2.12	0.49
1:A:109:VAL:CG2	1:A:138:GLN:HG3	2.43	0.49
1:A:225:PHE:CE2	1:A:277:ILE:HG23	2.47	0.49
1:A:569:SER:O	1:A:720:ALA:HB1	2.13	0.49
1:A:591:GLU:O	1:A:685:ARG:HB3	2.12	0.49
1:C:231:LYS:CG	1:C:232:LYS:N	2.75	0.49
2:F:451:VAL:CG1	2:F:451:VAL:O	2.61	0.49
1:A:191:THR:O	1:A:763:THR:HG22	2.12	0.49
2:B:516:LEU:O	2:B:545:PRO:HD2	2.12	0.49
1:C:360:PRO:HB2	1:C:363:ASP:HB2	1.94	0.49
1:C:485:VAL:O	1:C:485:VAL:HG22	2.12	0.49
1:E:296:ILE:O	1:E:300:LEU:HB2	2.12	0.49
1:E:70:ILE:HG22	1:E:388:THR:HG22	1.95	0.49
1:A:72:SER:HA	1:A:439:GLY:O	2.13	0.49
1:C:174:LEU:O	1:C:177:THR:HB	2.13	0.49
1:C:374:PRO:O	1:C:404:THR:HG23	2.11	0.49
2:D:505:ARG:HG3	2:D:505:ARG:NH1	2.28	0.49
1:E:211:PHE:N	1:E:211:PHE:CD2	2.80	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ASN:HB3	1:E:254:THR:OG1	2.12	0.49
1:E:784:LEU:HD23	1:E:794:PRO:CG	2.37	0.49
2:D:495:ASN:OD1	2:D:495:ASN:N	2.45	0.49
2:D:476:ALA:HA	2:D:582:LEU:HD23	1.93	0.49
1:A:258:THR:HG21	1:A:260:LYS:HG2	1.95	0.49
1:E:46:ILE:N	1:E:46:ILE:HD12	2.28	0.49
1:A:223:ARG:HG2	1:A:223:ARG:HH11	1.76	0.48
1:A:719:LEU:HD21	1:A:835:TRP:CD2	2.47	0.48
1:C:638:PRO:O	1:C:640:GLY:N	2.46	0.48
1:C:733:ILE:HG21	1:C:743:ILE:HD12	1.95	0.48
1:E:349:GLN:O	1:E:370:LYS:HA	2.12	0.48
2:F:467:ARG:HG3	2:F:558:TRP:CD1	2.48	0.48
1:C:543:GLN:O	1:C:546:GLU:N	2.46	0.48
1:C:734:GLN:HE21	1:C:734:GLN:N	2.11	0.48
1:E:381:TYR:OH	1:E:481:MET:HG3	2.13	0.48
1:E:4:PHE:HD1	1:E:8:GLN:OE1	1.95	0.48
1:E:524:GLU:HA	2:F:492:ARG:HH12	1.78	0.48
1:C:704:GLN:O	1:C:707:PRO:HD2	2.13	0.48
1:A:144:ARG:NH2	1:A:791:GLN:O	2.46	0.48
1:A:568:GLU:HB3	1:A:721:ASP:OD2	2.13	0.48
1:A:730:LEU:HB2	1:A:799:ASP:HB2	1.95	0.48
1:E:179:ALA:O	1:E:183:GLU:HB2	2.13	0.48
1:E:25:ILE:HG12	1:E:125:ALA:HB1	1.94	0.48
1:E:500:ASP:O	1:E:503:LYS:HB2	2.14	0.48
1:A:388:THR:HG21	1:A:395:TYR:CG	2.48	0.48
1:A:10:ARG:NH2	1:A:449:PRO:HD3	2.28	0.48
1:A:591:GLU:OE2	1:A:685:ARG:NH1	2.46	0.48
1:C:258:THR:HG22	1:C:260:LYS:N	2.26	0.48
1:E:69:THR:O	1:E:389:SER:N	2.44	0.48
1:E:699:DDE:HAB1	3:E:843:APR:O3A	2.14	0.48
2:F:552:LEU:CD1	2:F:552:LEU:N	2.75	0.48
2:F:457:ALA:HB2	2:F:558:TRP:CE3	2.49	0.48
1:A:106:PRO:CG	1:A:114:GLU:HG3	2.43	0.48
1:A:262:THR:HG22	1:A:267:LYS:O	2.14	0.48
1:A:711:ARG:HH11	2:B:577:ASN:HD21	1.62	0.48
1:C:706:ILE:HB	2:D:493:ILE:HD12	1.95	0.48
1:C:759:GLN:OE1	1:C:766:PHE:HE2	1.96	0.48
1:E:40:VAL:C	1:E:42:ARG:H	2.16	0.48
1:E:43:ALA:O	1:E:77:LEU:HA	2.14	0.48
1:E:699:DDE:HAA3	1:E:699:DDE:HAD2	1.77	0.48
1:A:132:ILE:HD12	1:A:162:ARG:HD3	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:TRP:HZ2	2:B:490:ARG:NH1	2.11	0.48
1:C:507:GLY:HA2	1:C:510:ARG:HD2	1.95	0.48
1:E:396:ALA:HB3	1:E:456:LEU:HB2	1.95	0.48
1:A:186:ASN:CB	1:A:201:GLN:HG2	2.44	0.48
1:C:106:PRO:CG	1:C:114:GLU:HG3	2.44	0.48
1:C:581:ASN:N	1:C:704:GLN:OE1	2.43	0.48
2:D:417:TRP:NE1	2:D:568:PRO:HB2	2.28	0.48
2:D:493:ILE:HG22	2:D:493:ILE:O	2.13	0.48
1:E:749:LYS:HG3	1:E:750:LYS:CD	2.44	0.48
1:A:118:ALA:O	1:A:122:THR:HG23	2.13	0.48
1:A:172:GLU:OE2	1:A:271:ARG:NH2	2.43	0.48
1:A:39:LEU:HB3	1:A:77:LEU:HD21	1.95	0.48
1:A:647:ILE:CG1	1:A:685:ARG:HE	2.25	0.48
1:A:669:TRP:HZ2	2:B:490:ARG:HH12	1.62	0.48
1:C:224:GLN:O	1:C:228:ARG:HG3	2.14	0.48
1:C:637:GLY:HA2	1:C:638:PRO:O	2.13	0.48
1:A:321:LYS:HZ2	1:A:325:ARG:HD3	1.78	0.48
1:A:466:THR:CG2	1:A:467:GLY:N	2.76	0.48
1:C:156:VAL:HG23	1:C:337:MET:HE1	1.95	0.48
1:C:223:ARG:HG2	1:C:223:ARG:NH1	2.29	0.48
1:C:208:THR:HG22	1:C:341:HIS:CG	2.49	0.48
2:D:465:ILE:CD1	2:D:465:ILE:H	2.25	0.48
1:E:552:VAL:HG13	1:E:553:PRO:N	2.28	0.48
1:E:699:DDE:HAC1	3:E:843:APR:H5'1	1.96	0.48
2:B:453:GLY:O	2:B:456:ARG:HD3	2.13	0.47
1:C:10:ARG:NH2	1:C:449:PRO:HD3	2.27	0.47
2:D:446:ALA:O	2:D:447:ALA:C	2.53	0.47
2:D:482:ALA:O	2:D:496:GLY:N	2.47	0.47
1:E:319:LEU:O	1:E:323:VAL:HG23	2.14	0.47
2:B:477:LEU:HB2	2:B:551:ARG:HD2	1.96	0.47
1:C:206:ARG:HG3	1:C:206:ARG:HH11	1.78	0.47
1:C:697:ALA:HA	1:C:700:ARG:CZ	2.44	0.47
1:E:749:LYS:O	1:E:750:LYS:HD2	2.14	0.47
1:E:727:PRO:HG2	1:E:774:VAL:HB	1.95	0.47
1:A:472:SER:HB3	1:A:475:ALA:HB2	1.96	0.47
2:B:502:TYR:HB2	2:B:565:VAL:O	2.14	0.47
1:C:186:ASN:HB3	1:C:201:GLN:HG2	1.97	0.47
1:E:167:LEU:HD12	1:E:167:LEU:N	2.29	0.47
1:E:220:PHE:HA	1:E:224:GLN:OE1	2.12	0.47
1:E:490:GLN:HA	1:E:531:ALA:HA	1.97	0.47
1:A:91:GLN:O	1:A:93:THR:HG23	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:LYS:O	1:C:513:LYS:HE3	2.14	0.47
2:D:552:LEU:HD12	2:D:552:LEU:N	2.29	0.47
1:E:307:LEU:HB2	1:E:312:LYS:CE	2.45	0.47
1:E:647:ILE:HB	1:E:687:ASN:ND2	2.30	0.47
1:A:149:GLU:HA	1:A:355:GLN:NE2	2.27	0.47
1:A:823:ARG:NH1	1:A:831:GLU:O	2.46	0.47
1:E:241:MET:HA	1:E:244:LEU:HD12	1.96	0.47
1:E:545:LEU:O	1:E:550:ALA:HB3	2.15	0.47
1:E:633:ILE:HD13	1:E:645:LEU:HD22	1.96	0.47
1:A:414:GLN:HB3	1:A:418:TYR:CD2	2.49	0.47
1:A:806:SER:HB2	1:A:813:SER:HB2	1.97	0.47
1:C:436:LEU:O	1:C:442:VAL:HA	2.14	0.47
1:E:82:SER:O	1:E:86:VAL:HG23	2.14	0.47
2:F:571:ILE:CD1	2:F:587:ILE:HD13	2.44	0.47
1:A:677:PHE:N	1:A:677:PHE:CD2	2.82	0.47
1:C:454:ILE:HG13	1:C:455:GLY:N	2.27	0.47
1:C:627:VAL:CG2	1:C:631:ARG:NH2	2.77	0.47
1:A:223:ARG:NH1	1:A:223:ARG:HG2	2.30	0.47
1:A:750:LYS:O	1:A:751:ARG:HB2	2.15	0.47
1:C:311:GLU:CA	1:C:314:LEU:HD13	2.40	0.47
1:E:153:PRO:HD2	1:E:200:VAL:HG22	1.97	0.47
1:E:488:VAL:HG23	1:E:489:VAL:HG23	1.96	0.47
1:E:4:PHE:HD1	1:E:8:GLN:CD	2.17	0.47
1:E:4:PHE:HA	1:E:8:GLN:OE1	2.15	0.47
1:A:16:VAL:CG1	1:A:345:PRO:HB2	2.45	0.47
1:C:100:ILE:HD13	1:C:338:ILE:HG21	1.96	0.47
1:C:468:THR:C	1:C:469:LEU:HD12	2.34	0.47
1:C:504:LEU:O	1:C:506:GLU:N	2.47	0.47
2:D:488:ASP:CG	2:D:489:ALA:N	2.68	0.47
2:D:566:VAL:HG12	2:D:567:ILE:N	2.30	0.47
1:E:677:PHE:CZ	1:E:679:GLU:HG3	2.50	0.47
1:E:740:VAL:HG21	1:E:766:PHE:CD1	2.49	0.47
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.15	0.47
1:A:488:VAL:HG23	1:A:489:VAL:HG23	1.96	0.47
1:E:225:PHE:CZ	1:E:328:LEU:HD11	2.50	0.47
1:A:12:LEU:HG	1:A:99:LEU:HB2	1.95	0.47
1:A:485:VAL:HG22	1:A:485:VAL:O	2.15	0.46
2:B:429:LEU:HD21	2:B:565:VAL:HG11	1.96	0.46
1:C:256:LYS:HA	1:C:256:LYS:CE	2.44	0.46
2:D:530:LEU:HD23	2:D:604:PRO:HD3	1.96	0.46
1:A:26:ALA:O	1:A:32:LYS:HD2	2.16	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:405:GLY:HA2	1:C:627:VAL:CG1	2.44	0.46
1:E:221:THR:OG1	1:E:224:GLN:HG3	2.15	0.46
1:A:103:ILE:HD13	1:A:121:VAL:HG23	1.97	0.46
1:A:189:VAL:CG1	1:A:200:VAL:HG12	2.45	0.46
1:A:511:LEU:HD22	1:A:545:LEU:HD13	1.96	0.46
1:C:385:MET:SD	1:C:396:ALA:HA	2.55	0.46
1:C:494:GLU:HA	1:C:494:GLU:OE1	2.14	0.46
1:E:397:PHE:HD1	1:E:437:MET:HG3	1.80	0.46
1:E:79:SER:O	1:E:98:PHE:N	2.47	0.46
2:F:443:PHE:CE2	2:F:445:GLU:HB2	2.50	0.46
1:A:685:ARG:NE	1:A:687:ASN:HD21	2.13	0.46
1:C:2:VAL:CG2	1:C:3:ALA:H	2.21	0.46
1:C:543:GLN:CG	1:C:544:ASP:N	2.74	0.46
1:C:567:VAL:HG23	1:C:592:PRO:HG3	1.97	0.46
2:D:551:ARG:HG3	2:D:551:ARG:NH1	2.31	0.46
1:E:383:SER:HA	1:E:481:MET:HE1	1.96	0.46
1:E:600:ALA:HB1	1:E:606:ILE:HG12	1.97	0.46
1:E:649:GLN:OE1	1:E:687:ASN:HB3	2.16	0.46
1:E:71:LYS:O	1:E:386:VAL:HG21	2.15	0.46
1:E:732:GLU:N	1:E:795:GLN:O	2.48	0.46
1:A:436:LEU:HD23	1:A:454:ILE:CD1	2.46	0.46
1:A:824:LYS:HE2	1:A:830:GLU:OE2	2.15	0.46
1:C:654:GLN:HG2	1:C:655:TYR:CD2	2.49	0.46
1:E:169:VAL:CG2	1:E:173:ASP:HB2	2.45	0.46
1:E:244:LEU:O	1:E:273:PHE:HB2	2.16	0.46
1:E:410:LYS:HA	1:E:430:ALA:HA	1.97	0.46
1:E:644:ASN:HD22	1:E:684:VAL:HB	1.81	0.46
1:E:804:LEU:N	1:E:804:LEU:HD23	2.30	0.46
1:A:338:ILE:O	1:A:342:LEU:HB2	2.16	0.46
1:A:565:GLU:O	1:A:681:MET:HA	2.16	0.46
2:B:563:ARG:HG3	2:B:563:ARG:NH1	2.31	0.46
1:C:231:LYS:HD3	1:C:232:LYS:H	1.80	0.46
1:E:237:LYS:O	1:E:241:MET:HG2	2.15	0.46
1:E:411:VAL:CG1	1:E:412:ARG:N	2.78	0.46
1:E:461:GLN:NE2	1:E:462:PHE:CE2	2.84	0.46
1:A:345:PRO:O	1:A:349:GLN:HG3	2.15	0.46
1:C:545:LEU:HA	1:C:549:HIS:HB2	1.98	0.46
2:D:465:ILE:N	2:D:465:ILE:HD13	2.29	0.46
2:D:447:ALA:HA	2:D:499:LEU:HD21	1.98	0.46
1:A:185:VAL:O	1:A:189:VAL:HG23	2.16	0.46
1:A:222:ILE:HD11	1:A:273:PHE:HE1	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:CYS:SG	1:A:739:ALA:HB3	2.56	0.46
2:B:479:TYR:CG	2:B:582:LEU:HB2	2.51	0.46
1:E:220:PHE:HB3	1:E:328:LEU:HD13	1.97	0.46
1:E:374:PRO:O	1:E:404:THR:HG23	2.16	0.46
2:F:520:ALA:HA	2:F:521:PRO:HD2	1.61	0.46
1:A:230:ALA:O	1:A:235:VAL:HG22	2.16	0.46
1:A:3:ALA:HA	1:A:46:ILE:HG22	1.96	0.46
2:B:417:TRP:NE1	2:B:568:PRO:HB2	2.31	0.46
2:B:435:VAL:HG11	2:B:508:LEU:HD11	1.97	0.46
1:C:739:ALA:HB2	1:C:791:GLN:OE1	2.16	0.46
2:D:538:ARG:HA	2:D:538:ARG:HD2	1.64	0.46
2:D:577:ASN:ND2	2:D:577:ASN:O	2.48	0.46
2:D:476:ALA:CA	2:D:582:LEU:HD23	2.46	0.46
1:E:129:VAL:HG13	1:E:135:VAL:HA	1.98	0.46
1:E:386:VAL:HA	1:E:387:PRO:HD3	1.78	0.46
1:E:528:HIS:O	1:E:529:ILE:HD13	2.16	0.46
1:E:685:ARG:HE	1:E:687:ASN:ND2	2.11	0.46
1:A:563:TYR:O	1:A:564:ARG:HD2	2.15	0.46
1:C:288:ILE:HG23	1:C:319:LEU:HG	1.98	0.46
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.97	0.46
1:C:742:GLY:O	1:C:745:SER:HB3	2.16	0.46
1:E:507:GLY:CA	1:E:549:HIS:HB3	2.46	0.46
1:E:728:VAL:HB	1:E:800:HIS:HD2	1.79	0.46
1:E:771:TYR:CE1	1:E:799:ASP:OD1	2.69	0.46
2:D:517:THR:HG21	2:D:548:GLU:N	2.31	0.45
1:E:108:HIS:HB2	1:E:111:PHE:CE2	2.52	0.45
1:E:202:VAL:O	1:E:202:VAL:HG23	2.16	0.45
1:E:21:ASN:ND2	1:E:345:PRO:HG3	2.31	0.45
2:F:517:THR:C	2:F:519:ALA:N	2.69	0.45
1:A:180:ARG:O	1:A:183:GLU:HB3	2.16	0.45
1:A:371:ASN:O	1:A:372:CYS:C	2.54	0.45
1:A:654:GLN:HG2	1:A:655:TYR:CG	2.51	0.45
1:C:110:ASP:C	1:C:112:SER:H	2.19	0.45
1:C:386:VAL:HA	1:C:387:PRO:HD3	1.87	0.45
1:C:406:LYS:HB3	1:C:447:ASP:CB	2.47	0.45
1:C:506:GLU:O	1:C:510:ARG:HG3	2.16	0.45
1:E:129:VAL:HG12	1:E:130:ASP:H	1.81	0.45
1:E:654:GLN:O	1:E:655:TYR:HB2	2.16	0.45
2:F:437:VAL:HG11	2:F:511:PHE:CE2	2.51	0.45
1:C:348:ALA:HA	1:C:351:TYR:CZ	2.51	0.45
1:C:459:ILE:O	1:C:462:PHE:N	2.48	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:ASP:OD1	1:C:691:VAL:N	2.48	0.45
1:E:112:SER:O	1:E:115:VAL:HB	2.17	0.45
1:E:239:LYS:O	1:E:239:LYS:HG2	2.16	0.45
2:F:500:ARG:O	2:F:566:VAL:HG13	2.16	0.45
2:F:538:ARG:HD2	2:F:538:ARG:HA	1.46	0.45
1:A:226:ALA:HB2	1:A:241:MET:HB3	1.97	0.45
1:A:228:ARG:C	1:A:230:ALA:H	2.18	0.45
1:A:400:VAL:O	1:A:450:ALA:HA	2.16	0.45
1:A:673:GLU:HG2	1:A:678:GLY:O	2.17	0.45
1:A:736:PRO:O	1:A:740:VAL:HG23	2.15	0.45
1:A:759:GLN:HB2	1:A:766:PHE:CE1	2.51	0.45
1:C:108:HIS:HD2	1:C:110:ASP:H	1.63	0.45
1:C:120:ARG:NH1	1:C:479:LYS:HG3	2.32	0.45
1:C:404:THR:CG2	1:C:449:PRO:HA	2.25	0.45
1:E:150:ARG:NH1	1:E:355:GLN:HB2	2.31	0.45
1:A:734:GLN:HE21	1:A:734:GLN:CA	2.26	0.45
1:C:111:PHE:HB3	1:C:114:GLU:HG2	1.99	0.45
1:C:335:LEU:O	1:C:339:VAL:HG23	2.16	0.45
2:D:427:ARG:O	2:D:430:GLU:N	2.48	0.45
1:E:158:ASN:HD22	1:E:159:LYS:HG3	1.81	0.45
1:E:117:ALA:HA	1:E:481:MET:SD	2.57	0.45
1:E:536:LEU:O	1:E:539:GLU:HB3	2.17	0.45
1:E:731:VAL:HG13	1:E:731:VAL:O	2.16	0.45
1:A:2:VAL:CG2	1:A:3:ALA:N	2.78	0.45
1:C:2:VAL:CG2	1:C:3:ALA:N	2.74	0.45
1:C:580:PRO:HD2	1:C:704:GLN:CD	2.37	0.45
2:D:429:LEU:HD21	2:D:565:VAL:HG11	1.98	0.45
1:E:171:LYS:NZ	1:E:283:ARG:HH21	2.14	0.45
1:E:39:LEU:C	1:E:39:LEU:HD23	2.36	0.45
1:E:454:ILE:CG1	1:E:455:GLY:N	2.79	0.45
1:E:581:ASN:HB3	1:E:583:HIS:CD2	2.50	0.45
1:A:160:VAL:HG23	1:A:212:GLY:O	2.17	0.45
1:A:73:THR:OG1	1:A:386:VAL:HG11	2.17	0.45
1:E:594:ASP:HB2	1:E:597:VAL:HG23	1.99	0.45
1:A:360:PRO:HD2	1:A:363:ASP:HB2	1.99	0.45
2:B:514:THR:OG1	2:B:515:SER:N	2.50	0.45
1:C:183:GLU:O	1:C:187:VAL:HG23	2.17	0.45
1:C:249:PHE:N	1:C:249:PHE:CD2	2.85	0.45
1:E:172:GLU:HA	1:E:274:ASN:HD21	1.81	0.45
1:E:391:LYS:CG	1:E:392:GLY:H	2.29	0.45
1:E:797:VAL:HG22	1:E:798:PHE:N	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:450:ILE:O	2:F:454:GLY:HA2	2.16	0.45
1:A:654:GLN:O	1:A:655:TYR:HB2	2.17	0.45
1:C:24:VAL:HG12	1:C:24:VAL:O	2.17	0.45
1:E:132:ILE:HD12	1:E:132:ILE:H	1.81	0.45
1:E:495:VAL:CG1	1:E:554:LEU:HD23	2.46	0.45
1:A:231:LYS:C	1:A:233:PHE:N	2.68	0.45
1:C:22:MET:HA	1:C:122:THR:HB	1.98	0.45
1:C:32:LYS:NZ	1:C:105:SER:HB2	2.32	0.45
1:C:76:SER:C	1:C:77:LEU:HD12	2.37	0.45
1:E:735:CYS:SG	1:E:739:ALA:HB3	2.56	0.45
1:A:249:PHE:CD2	1:A:249:PHE:N	2.85	0.44
1:A:40:VAL:C	1:A:42:ARG:H	2.21	0.44
1:C:82:SER:O	1:C:86:VAL:HG23	2.17	0.44
1:C:89:ILE:CG2	1:C:91:GLN:HG2	2.47	0.44
1:E:13:MET:SD	1:E:436:LEU:HD21	2.58	0.44
1:A:730:LEU:HD22	1:A:730:LEU:C	2.38	0.44
1:A:758:GLU:CG	1:A:767:THR:HG23	2.46	0.44
1:C:39:LEU:HB3	1:C:77:LEU:HD21	1.99	0.44
1:C:809:LEU:O	1:C:811:PRO:HD3	2.17	0.44
1:E:189:VAL:HG11	1:E:201:GLN:HA	1.99	0.44
1:E:68:ILE:HG21	1:E:395:TYR:OH	2.16	0.44
1:E:739:ALA:O	1:E:788:THR:HG22	2.17	0.44
1:E:792:ALA:O	1:E:794:PRO:HD3	2.17	0.44
2:F:400:PHE:CD1	2:F:429:LEU:CD2	3.00	0.44
1:A:110:ASP:C	1:A:112:SER:H	2.20	0.44
1:A:16:VAL:HG12	1:A:346:VAL:HG23	1.99	0.44
2:B:450:ILE:O	2:B:454:GLY:HA2	2.17	0.44
1:C:253:LYS:HG3	1:C:253:LYS:O	2.17	0.44
1:C:4:PHE:HD1	1:C:8:GLN:OE1	2.00	0.44
1:C:792:ALA:O	1:C:794:PRO:HD3	2.17	0.44
2:D:451:VAL:O	2:D:451:VAL:CG1	2.64	0.44
1:E:325:ARG:HH11	1:E:325:ARG:HG2	1.81	0.44
1:E:39:LEU:HD21	1:E:77:LEU:CG	2.47	0.44
1:E:3:ALA:HA	1:E:46:ILE:O	2.17	0.44
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.98	0.44
1:A:429:LYS:HG2	1:A:462:PHE:CE2	2.53	0.44
1:C:391:LYS:HE3	1:C:393:ARG:HG3	1.99	0.44
1:C:4:PHE:HD2	1:C:45:ILE:HG23	1.81	0.44
1:E:22:MET:HA	1:E:122:THR:HB	1.98	0.44
1:E:466:THR:HG22	1:E:467:GLY:N	2.32	0.44
1:E:533:THR:H	1:E:537:HIS:CD2	2.36	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:606:ILE:HD12	1:E:619:MET:HG2	2.00	0.44
1:E:759:GLN:HG2	1:E:760:ARG:N	2.32	0.44
1:A:112:SER:HB3	1:A:794:PRO:O	2.17	0.44
1:C:317:LYS:HD2	1:C:317:LYS:HA	1.66	0.44
1:C:836:GLN:N	1:C:836:GLN:HE21	2.03	0.44
1:E:25:ILE:HD12	1:E:142:VAL:HG12	1.99	0.44
1:E:690:ASP:O	1:E:691:VAL:HG23	2.18	0.44
1:A:117:ALA:HA	1:A:481:MET:SD	2.58	0.44
1:C:315:GLU:C	1:C:319:LEU:HB2	2.37	0.44
1:C:391:LYS:HE3	1:C:393:ARG:CG	2.48	0.44
1:E:733:ILE:HD13	1:E:743:ILE:HD12	2.00	0.44
1:E:760:ARG:O	1:E:761:PRO:C	2.56	0.44
1:E:699:DDE:CAB	3:E:843:APR:H5R1	2.47	0.44
1:A:296:ILE:N	1:A:297:PRO:HD2	2.32	0.44
1:A:580:PRO:HB2	1:A:704:GLN:HE22	1.83	0.44
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.98	0.44
2:B:436:PHE:HB2	2:B:502:TYR:CE2	2.53	0.44
1:C:336:GLU:HG2	1:C:340:LEU:HD12	2.00	0.44
1:E:171:LYS:HZ3	1:E:283:ARG:HH21	1.65	0.44
1:E:39:LEU:HD21	1:E:77:LEU:HD23	2.00	0.44
1:A:459:ILE:CD1	1:A:469:LEU:HD21	2.48	0.44
1:A:731:VAL:HG23	1:A:731:VAL:O	2.18	0.44
2:B:442:THR:OG1	2:B:443:PHE:N	2.51	0.44
1:C:200:VAL:O	1:C:200:VAL:HG13	2.17	0.44
1:C:222:ILE:HG22	1:C:241:MET:HB2	2.00	0.44
1:E:699:DDE:HAU2	1:E:699:DDE:HAC3	1.82	0.44
2:F:471:ILE:HG21	2:F:501:VAL:HG21	2.00	0.44
1:A:348:ALA:O	1:A:352:ARG:HB2	2.18	0.44
1:A:494:GLU:HB3	1:A:555:LYS:HB3	2.00	0.44
2:B:484:ASP:OD2	2:B:494:ARG:N	2.51	0.44
1:C:129:VAL:HG12	1:C:130:ASP:N	2.33	0.44
1:E:229:TYR:CE2	1:E:276:PHE:HB3	2.53	0.44
1:E:490:GLN:HB3	1:E:531:ALA:CB	2.41	0.44
2:F:505:ARG:NH1	2:F:505:ARG:CG	2.79	0.44
2:F:479:TYR:CG	2:F:582:LEU:HB2	2.53	0.44
1:A:231:LYS:C	1:A:233:PHE:H	2.19	0.43
1:A:45:ILE:HG12	1:A:76:SER:O	2.18	0.43
1:A:86:VAL:HG21	1:A:96:ASN:OD1	2.18	0.43
1:E:296:ILE:N	1:E:297:PRO:HD2	2.33	0.43
1:E:311:GLU:HA	1:E:314:LEU:CD1	2.47	0.43
1:A:730:LEU:CD2	1:A:730:LEU:C	2.87	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:VAL:C	1:C:18:ASN:N	2.72	0.43
2:D:490:ARG:O	2:D:492:ARG:N	2.52	0.43
1:E:341:HIS:O	1:E:342:LEU:C	2.57	0.43
1:E:485:VAL:HG22	1:E:485:VAL:O	2.18	0.43
2:F:517:THR:C	2:F:519:ALA:H	2.21	0.43
1:A:262:THR:HA	1:A:267:LYS:O	2.18	0.43
1:A:591:GLU:HG2	1:A:685:ARG:CG	2.47	0.43
1:A:634:TRP:CE3	1:A:660:LYS:HG3	2.53	0.43
1:C:251:ASN:HA	1:C:252:PRO:HD3	1.72	0.43
2:D:432:ARG:HA	2:D:432:ARG:NE	2.33	0.43
1:E:46:ILE:H	1:E:46:ILE:HD12	1.81	0.43
1:E:564:ARG:HD3	1:E:801:TRP:CH2	2.53	0.43
1:A:390:ASP:O	1:A:391:LYS:HB3	2.18	0.43
1:A:667:PHE:CZ	1:A:671:THR:HG21	2.53	0.43
2:B:446:ALA:O	2:B:447:ALA:C	2.56	0.43
1:C:283:ARG:HB3	1:C:299:LEU:HD21	2.00	0.43
2:D:451:VAL:O	2:D:451:VAL:HG12	2.17	0.43
1:E:536:LEU:CD1	1:E:540:ILE:HD11	2.48	0.43
1:E:620:ALA:HA	1:E:625:TRP:O	2.19	0.43
1:A:380:LEU:C	1:A:380:LEU:HD23	2.39	0.43
1:A:719:LEU:HD21	1:A:835:TRP:CE2	2.54	0.43
1:C:216:HIS:HB2	1:C:218:TRP:CD1	2.53	0.43
1:C:509:LYS:O	1:C:513:LYS:HG3	2.18	0.43
2:F:583:ASP:HA	2:F:584:PRO:HD2	1.89	0.43
1:C:524:GLU:C	1:C:526:GLY:H	2.21	0.43
2:D:490:ARG:HG3	2:D:490:ARG:O	2.19	0.43
1:E:21:ASN:ND2	1:E:345:PRO:CG	2.82	0.43
1:E:25:ILE:CG1	1:E:125:ALA:HB1	2.48	0.43
1:E:285:PHE:CD2	1:E:320:LEU:HD11	2.54	0.43
1:E:613:LYS:O	1:E:616:ALA:HB3	2.18	0.43
1:E:659:ILE:O	1:E:663:VAL:HG23	2.18	0.43
2:F:423:LEU:HD11	2:F:590:LYS:HD3	2.00	0.43
2:F:426:HIS:O	2:F:429:LEU:N	2.48	0.43
1:A:378:LEU:HD22	1:A:409:GLN:NE2	2.30	0.43
1:C:429:LYS:HE3	1:C:462:PHE:CE1	2.53	0.43
1:C:380:LEU:HB3	1:C:469:LEU:HB2	2.01	0.43
2:D:488:ASP:OD1	2:D:489:ALA:N	2.51	0.43
1:E:215:LEU:HD23	1:E:216:HIS:CE1	2.53	0.43
1:E:314:LEU:CD1	1:E:322:VAL:HG21	2.48	0.43
1:E:406:LYS:HB3	1:E:447:ASP:HB3	2.00	0.43
1:A:335:LEU:O	1:A:339:VAL:HG23	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ASN:O	1:A:615:ARG:HD3	2.19	0.43
1:E:303:LEU:O	1:E:304:GLU:CB	2.67	0.43
1:E:536:LEU:O	1:E:537:HIS:C	2.56	0.43
1:A:569:SER:O	1:A:592:PRO:HD3	2.18	0.43
1:A:581:ASN:O	1:A:582:LYS:CB	2.63	0.43
1:A:45:ILE:HB	1:A:76:SER:HB2	2.01	0.43
1:C:203:TYR:HB2	1:C:206:ARG:HB2	1.99	0.43
1:C:236:ASP:OD1	1:C:238:ALA:HB3	2.18	0.43
1:C:804:LEU:N	1:C:804:LEU:HD23	2.34	0.43
1:E:158:ASN:HA	1:E:212:GLY:O	2.19	0.43
1:E:225:PHE:CG	1:E:277:ILE:HD12	2.53	0.43
1:E:754:VAL:HA	1:E:770:ALA:HB2	2.01	0.43
1:E:784:LEU:CD2	1:E:794:PRO:HG3	2.40	0.43
1:E:699:DDE:HAB1	3:E:843:APR:H5'2	1.99	0.43
1:A:589:LYS:HE3	1:A:689:LEU:CD1	2.49	0.43
2:B:438:GLY:HA3	2:B:471:ILE:HD12	2.01	0.43
1:C:192:TYR:HA	1:C:763:THR:HG21	2.01	0.43
1:C:581:ASN:HB3	1:C:583:HIS:HB2	2.01	0.43
1:A:108:HIS:CD2	1:A:110:ASP:OD2	2.72	0.42
1:A:406:LYS:O	1:A:409:GLN:HB3	2.19	0.42
2:B:507:SER:C	2:B:509:PRO:HD2	2.39	0.42
1:C:26:ALA:CB	1:C:128:VAL:HB	2.48	0.42
1:C:504:LEU:C	1:C:506:GLU:N	2.72	0.42
1:C:558:PRO:HA	1:C:559:PRO:HD3	1.85	0.42
2:D:448:GLN:HB2	2:D:448:GLN:HE21	1.68	0.42
1:E:225:PHE:CD2	1:E:277:ILE:HD12	2.54	0.42
1:E:89:ILE:C	1:E:91:GLN:N	2.71	0.42
1:A:164:LEU:HD23	1:A:164:LEU:N	2.33	0.42
1:A:219:ALA:HB3	1:A:330:ALA:HA	2.01	0.42
1:A:411:VAL:CG1	1:A:412:ARG:N	2.81	0.42
1:C:217:GLY:HA3	1:C:325:ARG:NH1	2.34	0.42
1:C:497:ASN:N	1:C:497:ASN:ND2	2.66	0.42
2:D:447:ALA:O	2:D:448:GLN:C	2.57	0.42
1:E:493:VAL:HG22	1:E:556:ILE:HD12	2.00	0.42
1:E:690:ASP:OD1	1:E:691:VAL:N	2.46	0.42
1:E:699:DDE:HAB2	1:E:699:DDE:HAU3	1.71	0.42
2:F:450:ILE:O	2:F:454:GLY:N	2.52	0.42
1:A:363:ASP:O	1:A:367:ILE:HG13	2.19	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.81	0.42
1:C:237:LYS:O	1:C:241:MET:HG2	2.19	0.42
1:C:308:LYS:HB2	1:C:311:GLU:OE1	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:VAL:CG1	1:C:412:ARG:N	2.82	0.42
1:E:506:GLU:O	1:E:510:ARG:HG2	2.19	0.42
2:F:484:ASP:OD2	2:F:494:ARG:CG	2.66	0.42
1:A:37:ASP:O	1:A:40:VAL:N	2.52	0.42
1:C:253:LYS:CE	1:C:253:LYS:HA	2.28	0.42
1:C:718:LEU:HD12	1:C:718:LEU:HA	1.91	0.42
1:E:682:ARG:O	1:E:683:SER:HB2	2.20	0.42
1:A:42:ARG:HG2	1:A:331:ALA:HB1	2.01	0.42
2:B:523:ALA:O	2:B:524:ALA:C	2.56	0.42
1:C:19:VAL:HG12	1:C:20:ARG:N	2.35	0.42
1:C:220:PHE:HB3	1:C:328:LEU:HD13	2.01	0.42
1:C:218:TRP:CA	1:C:330:ALA:HB2	2.50	0.42
1:C:589:LYS:HE3	1:C:689:LEU:HD11	2.01	0.42
1:C:733:ILE:HG21	1:C:743:ILE:HD11	2.00	0.42
1:E:307:LEU:HB2	1:E:312:LYS:HD3	2.00	0.42
2:F:495:ASN:OD1	2:F:495:ASN:N	2.52	0.42
2:F:498:LEU:HD23	2:F:498:LEU:HA	1.72	0.42
1:A:200:VAL:O	1:A:200:VAL:CG1	2.67	0.42
1:A:682:ARG:O	1:A:683:SER:HB2	2.18	0.42
1:C:129:VAL:HG13	1:C:134:GLY:C	2.40	0.42
1:C:353:ALA:HB3	1:C:370:LYS:HG3	2.02	0.42
2:D:474:ASP:OD1	2:D:475:PRO:HD2	2.19	0.42
2:D:524:ALA:O	2:D:528:GLU:HG3	2.19	0.42
1:E:12:LEU:HG	1:E:99:LEU:HB2	2.02	0.42
1:A:390:ASP:O	1:A:391:LYS:CB	2.66	0.42
1:A:542:LEU:HD13	1:A:556:ILE:HG21	2.01	0.42
1:A:620:ALA:HA	1:A:625:TRP:O	2.19	0.42
1:A:810:ASP:O	1:A:816:GLY:HA3	2.20	0.42
2:D:530:LEU:HA	2:D:604:PRO:HG3	2.01	0.42
2:D:563:ARG:HD2	2:D:563:ARG:HA	1.86	0.42
1:E:153:PRO:HD2	1:E:200:VAL:CG2	2.49	0.42
1:E:89:ILE:HG23	1:E:340:LEU:O	2.19	0.42
1:E:493:VAL:HG12	1:E:494:GLU:N	2.34	0.42
2:F:426:HIS:CE1	2:F:594:ILE:HB	2.55	0.42
1:A:503:LYS:HB2	1:A:552:VAL:HG21	2.02	0.42
1:A:145:GLN:OE1	1:A:734:GLN:HG2	2.20	0.42
2:B:460:GLN:CB	2:B:467:ARG:HD3	2.49	0.42
1:C:727:PRO:HG2	1:C:774:VAL:HB	2.01	0.42
1:E:10:ARG:O	1:E:10:ARG:HD2	2.20	0.42
1:E:459:ILE:N	1:E:459:ILE:HD12	2.35	0.42
1:E:486:SER:HA	1:E:487:PRO:HD3	1.80	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:ASP:CG	1:E:552:VAL:HG21	2.40	0.42
1:E:578:LYS:HA	1:E:584:ASN:O	2.20	0.42
1:A:154:VAL:CG1	1:A:337:MET:HE3	2.50	0.42
1:A:380:LEU:HD23	1:A:381:TYR:N	2.35	0.42
1:A:491:VAL:HG13	1:A:538:LEU:HD21	2.02	0.42
2:B:511:PHE:CE1	2:B:560:LEU:HD11	2.55	0.42
1:C:146:ALA:O	1:C:151:ILE:HG12	2.19	0.42
1:C:13:MET:HB3	1:C:452:ASN:ND2	2.35	0.42
2:D:471:ILE:HG13	2:D:554:THR:HB	2.01	0.42
2:F:531:ILE:HG22	2:F:533:HIS:N	2.34	0.42
1:A:149:GLU:O	1:A:150:ARG:HB2	2.20	0.42
1:A:91:GLN:HE22	1:A:343:PRO:HA	1.84	0.42
1:A:644:ASN:HD22	1:A:684:VAL:N	2.14	0.42
1:A:192:TYR:HA	1:A:763:THR:CG2	2.50	0.42
1:C:384:LYS:CB	1:C:465:LYS:HE3	2.50	0.42
1:C:706:ILE:HB	1:C:707:PRO:HD3	2.01	0.42
1:C:799:ASP:OD1	1:C:800:HIS:CD2	2.70	0.42
1:E:606:ILE:HD12	1:E:619:MET:CG	2.50	0.42
1:E:677:PHE:N	1:E:677:PHE:CD2	2.88	0.42
1:E:39:LEU:CD2	1:E:77:LEU:CD2	2.97	0.42
2:F:456:ARG:HH21	2:F:458:ARG:NH2	2.16	0.42
1:C:228:ARG:C	1:C:230:ALA:H	2.24	0.41
1:E:306:VAL:O	1:E:306:VAL:HG23	2.20	0.41
1:E:406:LYS:O	1:E:409:GLN:HB3	2.18	0.41
2:F:446:ALA:O	2:F:447:ALA:C	2.59	0.41
2:F:540:ASP:N	2:F:540:ASP:OD2	2.51	0.41
1:A:387:PRO:HG3	1:A:394:PHE:CE1	2.55	0.41
1:A:487:PRO:HB3	1:A:531:ALA:HB1	2.03	0.41
1:A:89:ILE:CG2	1:A:91:GLN:HG2	2.50	0.41
1:C:131:THR:HG21	1:C:163:ALA:HB2	2.00	0.41
1:C:646:VAL:HG13	1:C:688:ILE:HD13	2.02	0.41
1:C:712:ALA:O	1:C:715:ALA:HB3	2.20	0.41
1:C:729:PHE:O	1:C:771:TYR:HA	2.20	0.41
1:C:784:LEU:CD2	1:C:794:PRO:HG3	2.40	0.41
2:D:484:ASP:OD2	2:D:494:ARG:CG	2.69	0.41
2:D:576:ARG:HH11	2:D:576:ARG:HG3	1.85	0.41
1:E:111:PHE:O	1:E:112:SER:C	2.57	0.41
1:E:143:LEU:O	1:E:147:LEU:HG	2.20	0.41
1:E:274:ASN:O	1:E:279:ASP:HB2	2.19	0.41
1:E:528:HIS:C	1:E:529:ILE:HD13	2.40	0.41
1:E:558:PRO:CB	1:E:559:PRO:HD2	2.49	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:677:PHE:HB3	1:E:819:VAL:HG13	2.01	0.41
1:E:749:LYS:C	1:E:750:LYS:HD2	2.41	0.41
2:F:505:ARG:C	2:F:507:SER:H	2.23	0.41
1:A:150:ARG:HG3	1:A:355:GLN:OE1	2.20	0.41
1:A:515:ASP:HA	1:A:516:PRO:HD3	1.88	0.41
1:C:291:PHE:CE1	1:C:316:GLY:N	2.89	0.41
2:D:507:SER:C	2:D:509:PRO:HD2	2.41	0.41
1:E:132:ILE:CD1	1:E:132:ILE:N	2.83	0.41
1:E:338:ILE:HA	1:E:342:LEU:HG	2.02	0.41
1:E:21:ASN:HD22	1:E:345:PRO:HG3	1.85	0.41
1:A:125:ALA:HB2	1:A:151:ILE:HG21	2.02	0.41
1:A:211:PHE:O	1:A:219:ALA:HA	2.19	0.41
1:A:380:LEU:HD13	1:A:456:LEU:HD11	2.01	0.41
1:C:275:MET:HE1	1:C:276:PHE:CZ	2.55	0.41
1:C:619:MET:HA	1:C:623:TYR:HD2	1.84	0.41
1:C:784:LEU:HD23	1:C:794:PRO:CG	2.41	0.41
1:E:202:VAL:HB	1:E:209:VAL:CG2	2.50	0.41
1:E:164:LEU:HD12	1:E:285:PHE:CE1	2.56	0.41
1:E:412:ARG:HG2	1:E:412:ARG:NH1	2.35	0.41
1:E:823:ARG:HH12	1:E:828:MET:CB	2.33	0.41
1:A:27:HIS:HD2	1:A:29:ASP:N	2.09	0.41
1:A:677:PHE:N	1:A:677:PHE:HD2	2.18	0.41
1:A:739:ALA:C	1:A:741:GLY:N	2.74	0.41
1:C:296:ILE:N	1:C:297:PRO:HD2	2.36	0.41
1:C:319:LEU:O	1:C:323:VAL:HG23	2.21	0.41
1:C:539:GLU:O	1:C:542:LEU:HB2	2.21	0.41
1:C:823:ARG:NH1	1:C:823:ARG:HG2	2.34	0.41
1:C:823:ARG:NH1	1:C:828:MET:HB2	2.35	0.41
1:E:411:VAL:HG13	1:E:470:THR:O	2.20	0.41
1:E:663:VAL:HG13	1:E:709:MET:SD	2.61	0.41
2:F:487:PRO:N	2:F:493:ILE:HD11	2.36	0.41
1:A:109:VAL:HG22	1:A:138:GLN:HG3	2.03	0.41
1:A:550:ALA:C	1:A:552:VAL:H	2.24	0.41
2:B:577:ASN:HD22	2:B:577:ASN:C	2.24	0.41
1:C:140:GLU:HG3	1:C:188:ILE:HD11	1.97	0.41
1:C:530:VAL:O	1:C:538:LEU:HD11	2.20	0.41
1:C:626:ASP:O	1:C:627:VAL:C	2.58	0.41
1:C:81:MET:O	1:C:96:ASN:HB3	2.21	0.41
1:E:468:THR:C	1:E:469:LEU:HD12	2.41	0.41
2:F:476:ALA:N	2:F:582:LEU:HD23	2.35	0.41
1:C:288:ILE:CG2	1:C:319:LEU:HG	2.50	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.88	0.41
1:E:336:GLU:HG2	1:E:340:LEU:HD12	2.01	0.41
1:E:591:GLU:CG	1:E:685:ARG:HG2	2.51	0.41
1:A:220:PHE:C	1:A:220:PHE:CD1	2.94	0.41
1:A:270:GLU:OE1	1:A:275:MET:HG3	2.21	0.41
2:B:503:VAL:HG12	2:B:564:THR:HG22	2.02	0.41
1:C:166:GLU:HB3	1:C:167:LEU:H	1.63	0.41
1:C:3:ALA:HA	1:C:46:ILE:HG22	2.02	0.41
1:C:406:LYS:O	1:C:409:GLN:HB3	2.21	0.41
1:C:600:ALA:HB1	1:C:606:ILE:HG12	2.02	0.41
1:C:682:ARG:O	1:C:683:SER:HB2	2.20	0.41
1:E:307:LEU:HB2	1:E:312:LYS:CD	2.51	0.41
1:E:436:LEU:HD23	1:E:454:ILE:CD1	2.51	0.41
1:E:807:ASP:HA	1:E:808:PRO:HD2	1.96	0.41
2:F:435:VAL:HG21	2:F:598:PRO:HG3	2.03	0.41
1:A:192:TYR:HA	1:A:763:THR:HG21	2.03	0.41
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.85	0.41
1:A:522:MET:CE	1:A:526:GLY:O	2.68	0.41
1:C:124:GLY:HA3	1:C:342:LEU:HD22	2.02	0.41
1:C:627:VAL:HG22	1:C:631:ARG:CZ	2.50	0.41
1:E:360:PRO:C	1:E:362:ASP:H	2.23	0.41
1:E:515:ASP:HA	1:E:516:PRO:HD3	1.80	0.41
1:A:153:PRO:HD2	1:A:200:VAL:CG1	2.51	0.41
1:A:186:ASN:CG	1:A:201:GLN:HG2	2.42	0.41
1:A:634:TRP:O	1:A:635:CYS:HB3	2.20	0.41
1:A:705:ILE:O	1:A:706:ILE:C	2.59	0.41
1:C:153:PRO:HD2	1:C:200:VAL:HG13	2.03	0.41
1:C:18:ASN:ND2	1:C:98:PHE:CE1	2.89	0.41
1:E:195:GLU:H	1:E:195:GLU:HG3	1.66	0.41
1:E:218:TRP:HA	1:E:328:LEU:O	2.21	0.41
1:E:357:TYR:CE2	1:E:359:GLY:HA3	2.56	0.41
1:E:654:GLN:HG2	1:E:655:TYR:CD2	2.55	0.41
1:E:731:VAL:CG2	1:E:796:MET:HB3	2.51	0.41
2:F:558:TRP:HA	2:F:561:ALA:HB3	2.02	0.41
1:A:167:LEU:N	1:A:167:LEU:HD12	2.36	0.41
1:A:285:PHE:CE2	1:A:320:LEU:HD11	2.56	0.41
1:A:4:PHE:CE2	1:A:45:ILE:HD12	2.55	0.41
1:A:600:ALA:HB1	1:A:606:ILE:HG13	2.03	0.41
2:B:535:LEU:HB3	2:B:536:PRO:HA	2.03	0.41
1:C:384:LYS:HB2	1:C:465:LYS:CE	2.51	0.41
1:C:612:PHE:HA	1:C:615:ARG:NH2	2.36	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:498:LEU:HA	2:D:498:LEU:HD23	1.72	0.41
1:E:77:LEU:HD22	1:E:100:ILE:HG22	2.03	0.41
2:F:410:SER:OG	2:F:412:ARG:HB2	2.21	0.41
2:F:470:TYR:CD2	2:F:555:ILE:HG12	2.56	0.41
1:C:413:ILE:HD13	1:C:459:ILE:HG23	2.03	0.40
1:C:109:VAL:HG13	1:C:793:PHE:HE1	1.86	0.40
1:E:735:CYS:HA	1:E:736:PRO:HD3	1.86	0.40
1:A:549:HIS:CD2	1:A:549:HIS:H	2.38	0.40
2:B:448:GLN:HE21	2:B:448:GLN:HB2	1.63	0.40
1:C:400:VAL:O	1:C:451:GLY:N	2.39	0.40
1:C:10:ARG:CZ	1:C:449:PRO:HD3	2.52	0.40
1:C:490:GLN:O	1:C:491:VAL:CG1	2.68	0.40
1:E:144:ARG:HG2	1:E:192:TYR:CG	2.56	0.40
1:E:155:VAL:HB	1:E:209:VAL:HG22	2.03	0.40
2:F:505:ARG:O	2:F:507:SER:N	2.54	0.40
1:A:231:LYS:O	1:A:233:PHE:N	2.55	0.40
1:A:254:THR:O	1:A:255:LYS:HB2	2.21	0.40
1:A:13:MET:HB3	1:A:452:ASN:ND2	2.37	0.40
1:A:504:LEU:HD13	1:A:554:LEU:HD21	2.02	0.40
2:B:531:ILE:HD12	2:B:533:HIS:CE1	2.56	0.40
2:D:448:GLN:O	2:D:449:SER:C	2.60	0.40
1:E:225:PHE:HZ	1:E:328:LEU:HD11	1.85	0.40
1:E:414:GLN:HB3	1:E:418:TYR:CD2	2.56	0.40
1:E:496:LYS:HB2	1:E:555:LYS:HZ3	1.86	0.40
1:E:601:ILE:HG12	1:E:606:ILE:HB	2.04	0.40
1:E:68:ILE:HD12	1:E:390:ASP:CB	2.27	0.40
1:A:429:LYS:CG	1:A:430:ALA:N	2.78	0.40
2:B:492:ARG:HG2	2:B:492:ARG:O	2.21	0.40
1:C:536:LEU:O	1:C:540:ILE:HG12	2.22	0.40
1:C:840:ASP:CG	1:C:842:LEU:HD13	2.41	0.40
1:E:158:ASN:O	1:E:159:LYS:HB2	2.21	0.40
1:E:188:ILE:HG23	1:E:192:TYR:CE2	2.57	0.40
1:E:27:HIS:CD2	1:E:28:VAL:N	2.89	0.40
1:E:305:ILE:HG21	1:E:323:VAL:HG13	2.03	0.40
1:E:617:ARG:NE	1:E:617:ARG:HA	2.37	0.40
2:F:528:GLU:OE2	2:F:535:LEU:N	2.42	0.40
2:F:566:VAL:HG12	2:F:567:ILE:N	2.37	0.40
1:A:212:GLY:HA2	1:A:218:TRP:CZ3	2.57	0.40
1:A:321:LYS:HZ2	1:A:325:ARG:HH11	1.70	0.40
1:A:581:ASN:ND2	1:A:699:DDE:O	2.55	0.40
1:C:284:LEU:HD23	1:C:299:LEU:HG	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:611:ASP:O	1:C:612:PHE:C	2.60	0.40
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.86	0.40
1:C:636:PHE:CE1	1:C:645:LEU:HD21	2.56	0.40
1:C:73:THR:HG22	1:C:73:THR:O	2.21	0.40
1:E:149:GLU:O	1:E:150:ARG:HB2	2.21	0.40
1:E:581:ASN:ND2	1:E:699:DDE:O	2.53	0.40
1:E:595:GLU:OE2	1:E:682:ARG:NH1	2.49	0.40
2:F:429:LEU:HD13	2:F:502:TYR:CG	2.56	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	818/842 (97%)	732 (90%)	74 (9%)	12 (2%)	10	37
1	C	818/842 (97%)	711 (87%)	87 (11%)	20 (2%)	6	25
1	E	818/842 (97%)	707 (86%)	97 (12%)	14 (2%)	9	34
2	B	205/207 (99%)	179 (87%)	24 (12%)	2 (1%)	15	47
2	D	205/207 (99%)	176 (86%)	24 (12%)	5 (2%)	6	25
2	F	205/207 (99%)	175 (85%)	27 (13%)	3 (2%)	10	37
All	All	3069/3147 (98%)	2680 (87%)	333 (11%)	56 (2%)	8	32

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	SER
1	C	235	VAL
1	C	460	ASP
1	C	639	ASP

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	761	PRO
1	E	112	SER
1	E	761	PRO
1	A	309	GLY
1	A	460	ASP
1	A	498	ALA
1	A	761	PRO
2	B	518	LEU
1	C	309	GLY
2	D	491	GLY
1	E	304	GLU
1	E	390	ASP
1	E	428	ILE
1	E	479	LYS
1	E	621	ASP
2	F	506	SER
1	A	479	LYS
2	B	506	SER
1	C	112	SER
1	C	314	LEU
1	C	479	LYS
1	C	582	LYS
2	D	405	GLY
1	E	233	PHE
2	F	577	ASN
1	A	111	PHE
1	A	215	LEU
1	A	390	ASP
1	A	610	ASP
1	C	329	PRO
1	C	390	ASP
1	C	446	ASP
2	D	447	ALA
1	E	302	LYS
1	E	582	LYS
1	E	743	ILE
1	A	287	ALA
1	A	391	LYS
1	C	166	GLU
1	C	266	GLY
1	C	505	VAL
1	E	446	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	460	ASP
1	C	292	LYS
1	C	558	PRO
1	C	677	PHE
1	E	90	LYS
1	C	491	VAL
1	C	743	ILE
2	D	454	GLY
2	D	604	PRO
2	F	493	ILE

### 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	699/714 (98%)	669 (96%)	30 (4%)	29	60
1	C	699/714 (98%)	651 (93%)	48 (7%)	15	44
1	E	699/714 (98%)	664 (95%)	35 (5%)	24	55
2	B	161/162 (99%)	145 (90%)	16 (10%)	8	27
2	D	161/162 (99%)	144 (89%)	17 (11%)	6	24
2	F	161/162 (99%)	146 (91%)	15 (9%)	9	31
All	All	2580/2628 (98%)	2419 (94%)	161 (6%)	18	48

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	28	VAL
1	A	81	MET
1	A	83	ASP
1	A	94	ASP
1	A	112	SER
1	A	138	GLN
1	A	152	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	195	GLU
1	A	200	VAL
1	A	236	ASP
1	A	262	THR
1	A	275	MET
1	A	347	THR
1	A	352	ARG
1	A	429	LYS
1	A	460	ASP
1	A	544	ASP
1	A	599	LEU
1	A	677	PHE
1	A	698	ILE
1	A	710	ARG
1	A	718	LEU
1	A	730	LEU
1	A	734	GLN
1	A	738	GLN
1	A	767	THR
1	A	775	ASN
1	A	836	GLN
1	A	842	LEU
2	B	412	ARG
2	B	422	LEU
2	B	448	GLN
2	B	467	ARG
2	B	488	ASP
2	B	492	ARG
2	B	494	ARG
2	B	495	ASN
2	B	499	LEU
2	B	518	LEU
2	B	540	ASP
2	B	547	GLU
2	B	551	ARG
2	B	560	LEU
2	B	577	ASN
2	B	602	SER
1	C	14	ASP
1	C	23	SER
1	C	28	VAL
1	C	36	THR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	81	MET
1	C	83	ASP
1	C	94	ASP
1	C	105	SER
1	C	164	LEU
1	C	183	GLU
1	C	195	GLU
1	C	200	VAL
1	C	231	LYS
1	C	242	ASP
1	C	253	LYS
1	C	320	LEU
1	C	347	THR
1	C	352	ARG
1	C	432	GLN
1	C	460	ASP
1	C	461	GLN
1	C	489	VAL
1	C	494	GLU
1	C	495	VAL
1	C	500	ASP
1	C	524	GLU
1	C	528	HIS
1	C	543	GLN
1	C	544	ASP
1	C	552	VAL
1	C	556	ILE
1	C	599	LEU
1	C	609	ARG
1	C	625	TRP
1	C	634	TRP
1	C	677	PHE
1	C	718	LEU
1	C	730	LEU
1	C	734	GLN
1	C	738	GLN
1	C	757	GLU
1	C	761	PRO
1	C	767	THR
1	C	775	ASN
1	C	813	SER
1	C	820	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	836	GLN
1	C	837	GLU
2	D	403	ASP
2	D	411	THR
2	D	422	LEU
2	D	465	ILE
2	D	467	ARG
2	D	483	GLN
2	D	488	ASP
2	D	494	ARG
2	D	499	LEU
2	D	538	ARG
2	D	540	ASP
2	D	547	GLU
2	D	551	ARG
2	D	560	LEU
2	D	577	ASN
2	D	602	SER
2	D	604	PRO
1	E	77	LEU
1	E	94	ASP
1	E	161	ASP
1	E	186	ASN
1	E	194	ASP
1	E	211	PHE
1	E	216	HIS
1	E	263	ASP
1	E	275	MET
1	E	282	PHE
1	E	313	ASP
1	E	347	THR
1	E	362	ASP
1	E	440	ARG
1	E	460	ASP
1	E	544	ASP
1	E	552	VAL
1	E	599	LEU
1	E	625	TRP
1	E	627	VAL
1	E	634	TRP
1	E	677	PHE
1	E	685	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	698	ILE
1	E	710	ARG
1	E	718	LEU
1	E	730	LEU
1	E	734	GLN
1	E	761	PRO
1	E	767	THR
1	E	786	GLN
1	E	800	HIS
1	E	823	ARG
1	E	836	GLN
1	E	837	GLU
2	F	411	THR
2	F	422	LEU
2	F	437	VAL
2	F	498	LEU
2	F	499	LEU
2	F	513	ARG
2	F	514	THR
2	F	538	ARG
2	F	540	ASP
2	F	547	GLU
2	F	548	GLU
2	F	552	LEU
2	F	560	LEU
2	F	577	ASN
2	F	604	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	HIS
1	A	91	GLN
1	A	108	HIS
1	A	138	GLN
1	A	201	GLN
1	A	371	ASN
1	A	409	GLN
1	A	452	ASN
1	A	537	HIS
1	A	549	HIS
1	A	581	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	583	HIS
1	A	584	ASN
1	A	644	ASN
1	A	654	GLN
1	A	687	ASN
1	A	694	HIS
1	A	734	GLN
1	A	738	GLN
1	A	753	GLN
1	A	800	HIS
1	A	836	GLN
2	B	428	GLN
2	B	448	GLN
2	B	495	ASN
2	B	577	ASN
1	C	21	ASN
1	C	27	HIS
1	C	91	GLN
1	C	138	GLN
1	C	201	GLN
1	C	251	ASN
1	C	259	ASN
1	C	274	ASN
1	C	414	GLN
1	C	452	ASN
1	C	497	ASN
1	C	528	HIS
1	C	537	HIS
1	C	547	HIS
1	C	549	HIS
1	C	581	ASN
1	C	583	HIS
1	C	584	ASN
1	C	644	ASN
1	C	694	HIS
1	C	734	GLN
1	C	738	GLN
1	C	753	GLN
1	C	759	GLN
1	C	800	HIS
1	C	836	GLN
2	D	428	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	448	GLN
2	D	460	GLN
2	D	577	ASN
1	E	27	HIS
1	E	91	GLN
1	E	138	GLN
1	E	201	GLN
1	E	371	ASN
1	E	537	HIS
1	E	581	ASN
1	E	583	HIS
1	E	584	ASN
1	E	644	ASN
1	E	687	ASN
1	E	694	HIS
1	E	734	GLN
1	E	753	GLN
1	E	800	HIS
1	E	836	GLN
2	F	448	GLN
2	F	460	GLN
2	F	577	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	DDE	C	699	1	5,10,21	1.22	1 (20%)	3,12,30	1.25	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	DDE	E	699	1,3	14,20,21	2.05	4 (28%)	14,28,30	2.40	4 (28%)
1	DDE	A	699	1	5,10,21	0.80	0	3,12,30	1.26	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DDE	C	699	1	-	1/5/6/23	0/1/1/1
1	DDE	E	699	1,3	-	2/20/21/23	0/1/1/1
1	DDE	A	699	1	-	1/5/6/23	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	699	DDE	OAG-CBI	4.98	1.33	1.23
1	E	699	DDE	CAT-CE1	3.61	1.55	1.50
1	E	699	DDE	CAC-NCB	2.89	1.59	1.50
1	C	699	DDE	CB-CA	2.17	1.58	1.53
1	E	699	DDE	CBW-CBI	2.04	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	699	DDE	OAG-CBI-CBW	-6.21	112.63	120.49
1	E	699	DDE	OAG-CBI-NAD	4.73	131.24	123.00
1	E	699	DDE	CE1-ND1-CG	2.18	109.51	103.05
1	E	699	DDE	CAT-CE1-ND1	2.18	128.63	122.54
1	A	699	DDE	CD2-NE2-CE1	2.05	108.97	105.78
1	C	699	DDE	CD2-NE2-CE1	2.02	108.93	105.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	699	DDE	O-C-CA-CB
1	E	699	DDE	CAU-CAT-CE1-ND1
1	E	699	DDE	CE1-CAT-CAU-CBW
1	A	699	DDE	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	699	DDE	1	0
1	E	699	DDE	11	0
1	A	699	DDE	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	APR	E	843	1	33,38,39	1.47	6 (18%)	37,58,60	1.76	7 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	APR	E	843	1	1/1/9/10	3/18/51/54	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	843	APR	C2-N1	4.17	1.41	1.33
3	E	843	APR	C3'-C4'	2.91	1.60	1.53
3	E	843	APR	O2'-C2'	2.73	1.49	1.43
3	E	843	APR	C4-N3	2.28	1.38	1.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	843	APR	O4D-C4D	2.24	1.48	1.44
3	E	843	APR	O4D-C1D	2.11	1.48	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	843	APR	O2D-C2D-C3D	-4.95	101.89	111.27
3	E	843	APR	PB-O3A-PA	-4.10	118.74	132.83
3	E	843	APR	C1D-C2D-C3D	3.77	107.37	101.63
3	E	843	APR	C1D-O4D-C4D	3.23	115.71	108.16
3	E	843	APR	O4D-C1D-C2D	-2.74	100.68	105.99
3	E	843	APR	C5-C6-N6	2.66	124.39	120.35
3	E	843	APR	C3'-C2'-C1'	2.43	104.64	100.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	843	APR	C1D

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	843	APR	C3'-C4'-C5'-O5'
3	E	843	APR	O4'-C4'-C5'-O5'
3	E	843	APR	C5D-O5D-PB-O1B

There are no ring outliers.

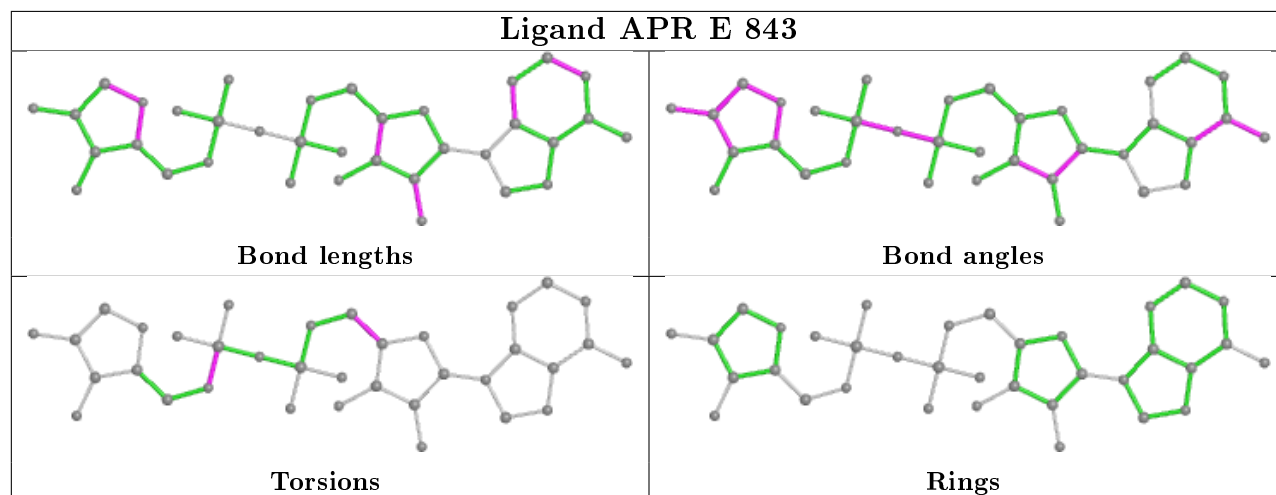
1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	843	APR	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and



any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 ⓘ

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	822/842 (97%)	-0.44	0	100	100	5, 48, 81, 101	0
1	C	822/842 (97%)	-0.13	24 (2%)	51	27	11, 64, 123, 135	0
1	E	822/842 (97%)	0.53	106 (12%)	3	1	7, 106, 129, 147	0
2	B	207/207 (100%)	-0.72	0	100	100	5, 22, 55, 71	0
2	D	207/207 (100%)	-0.65	0	100	100	5, 25, 64, 78	0
2	F	207/207 (100%)	-0.64	0	100	100	7, 27, 64, 79	0
All	All	3087/3147 (98%)	-0.14	130 (4%)	36	18	5, 54, 123, 147	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	269	LEU	5.5
1	E	197	LEU	5.2
1	E	167	LEU	5.2
1	C	499	ASN	5.0
1	E	166	GLU	4.9
1	E	163	ALA	4.8
1	E	231	LYS	4.7
1	E	314	LEU	4.6
1	E	195	GLU	4.4
1	E	737	GLU	4.3
1	E	194	ASP	4.3
1	E	759	GLN	4.3
1	E	175	TYR	4.3
1	E	313	ASP	4.1
1	E	257	TRP	4.0
1	E	110	ASP	4.0
1	E	107	GLY	4.0
1	E	201	GLN	3.9
1	E	132	ILE	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	67	GLY	3.9
1	E	258	THR	3.8
1	C	551	GLY	3.8
1	E	33	SER	3.8
1	C	270	GLU	3.8
1	E	193	ALA	3.7
1	E	196	VAL	3.6
1	E	444	PRO	3.6
1	E	254	THR	3.5
1	C	552	VAL	3.5
1	E	317	LYS	3.5
1	E	200	VAL	3.4
1	E	240	MET	3.4
1	C	167	LEU	3.2
1	E	189	VAL	3.2
1	E	108	HIS	3.1
1	E	276	PHE	3.1
1	E	32	LYS	3.1
1	E	245	TRP	3.1
1	C	260	LYS	3.1
1	E	777	SER	3.0
1	E	230	ALA	3.0
1	E	48	ALA	3.0
1	E	541	CYS	3.0
1	E	510	ARG	2.9
1	E	359	GLY	2.9
1	E	420	PRO	2.9
1	E	80	GLU	2.9
1	E	310	ASP	2.9
1	E	551	GLY	2.9
1	E	302	LYS	2.8
1	E	155	VAL	2.8
1	E	421	GLY	2.8
1	E	47	SER	2.8
1	E	307	LEU	2.8
1	E	104	ASP	2.8
1	E	309	GLY	2.7
1	E	554	LEU	2.7
1	E	36	THR	2.7
1	E	179	ALA	2.7
1	E	367	ILE	2.7
1	E	790	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	770	ALA	2.7
1	E	158	ASN	2.7
1	E	498	ALA	2.7
1	E	268	PRO	2.6
1	E	316	GLY	2.6
1	E	146	ALA	2.6
1	C	251	ASN	2.6
1	C	497	ASN	2.6
1	C	266	GLY	2.5
1	E	335	LEU	2.5
1	C	300	LEU	2.5
1	E	277	ILE	2.5
1	E	755	VAL	2.5
1	C	291	PHE	2.5
1	E	525	SER	2.5
1	C	544	ASP	2.5
1	E	262	THR	2.4
1	E	187	VAL	2.4
1	E	280	PRO	2.4
1	C	548	ASP	2.4
1	E	221	THR	2.4
1	C	307	LEU	2.4
1	E	362	ASP	2.4
1	E	757	GLU	2.4
1	E	559	PRO	2.4
1	E	333	ALA	2.4
1	E	398	GLY	2.4
1	E	308	LYS	2.4
1	E	499	ASN	2.4
1	E	256	LYS	2.4
1	E	216	HIS	2.4
1	E	290	ASN	2.3
1	C	3	ALA	2.3
1	E	205	ALA	2.3
1	E	232	LYS	2.3
1	E	781	THR	2.3
1	C	554	LEU	2.3
1	C	216	HIS	2.3
1	E	294	ASP	2.3
1	E	315	GLU	2.3
1	E	758	GLU	2.2
1	E	267	LYS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	34	THR	2.2
1	E	264	ALA	2.2
1	E	261	ASP	2.2
1	C	265	GLU	2.2
1	E	78	TYR	2.2
1	E	97	SER	2.2
1	E	503	LYS	2.2
1	C	302	LYS	2.2
1	E	88	GLU	2.1
1	E	360	PRO	2.1
1	C	496	LYS	2.1
1	E	311	GLU	2.1
1	E	745	SER	2.1
1	E	21	ASN	2.1
1	E	28	VAL	2.1
1	C	261	ASP	2.1
1	C	310	ASP	2.1
1	E	390	ASP	2.1
1	E	349	GLN	2.1
1	E	255	LYS	2.1
1	E	501	LEU	2.1
1	E	131	THR	2.0
1	E	212	GLY	2.0
1	C	263	ASP	2.0
1	E	168	GLN	2.0
1	C	268	PRO	2.0
1	E	354	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	DDE	C	699	10/21	0.84	0.21	44,52,55,56	0
1	DDE	A	699	10/21	0.89	0.12	37,41,46,47	0
1	DDE	E	699	20/21	0.92	0.29	48,68,80,81	0

## 6.3 Carbohydrates [i](#)

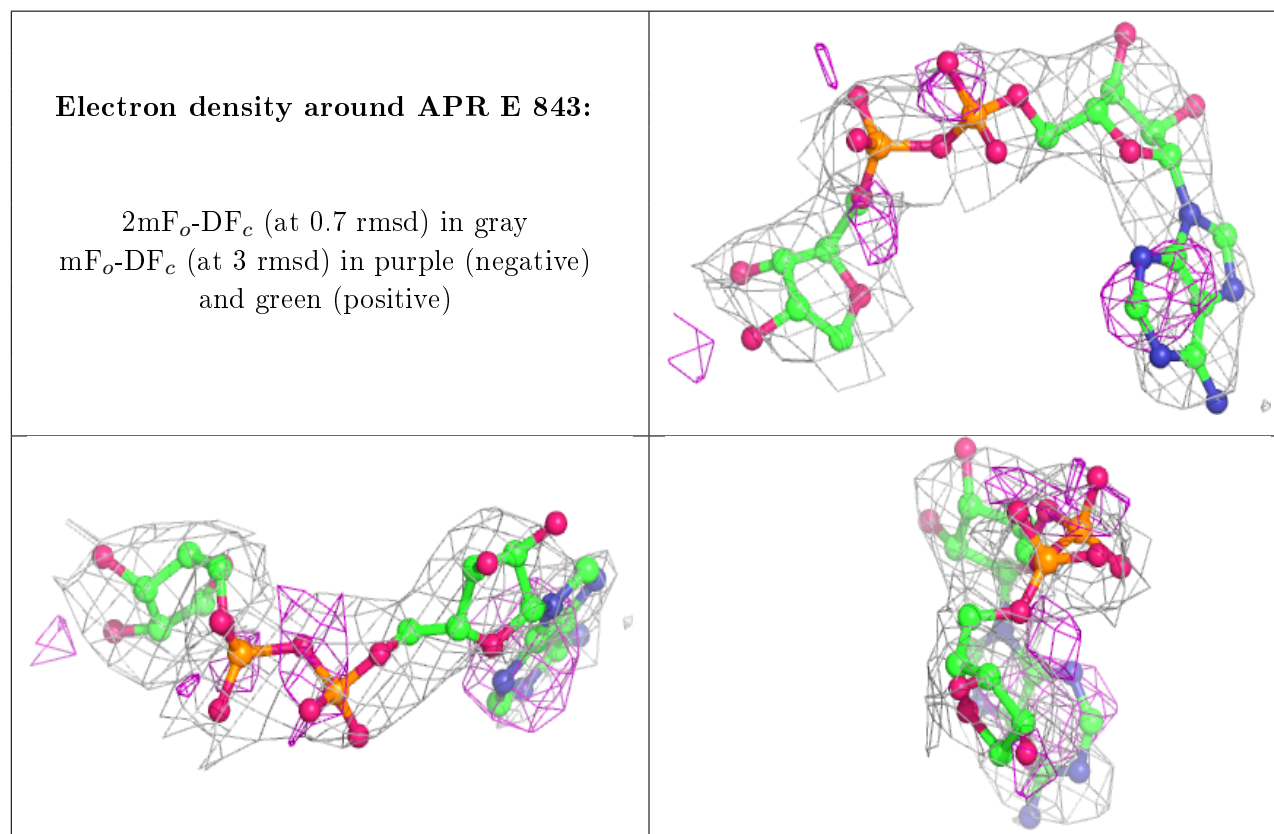
There are no carbohydrates in this entry.

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	APR	E	843	35/36	0.85	0.33	64,71,85,86	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.