



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 21, 2024 – 06:41 AM EDT

PDB ID : 2G63
Title : Crystal structure of human dipeptidyl peptidase IV (DPPIV) complexed with cyanopyrrolidine (C5-pro-pro) inhibitor 24b
Authors : Longenecker, K.L.; Fry, E.H.; Lake, M.R.; Solomon, L.R.; Pei, Z.; Li, X.
Deposited on : 2006-02-24
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

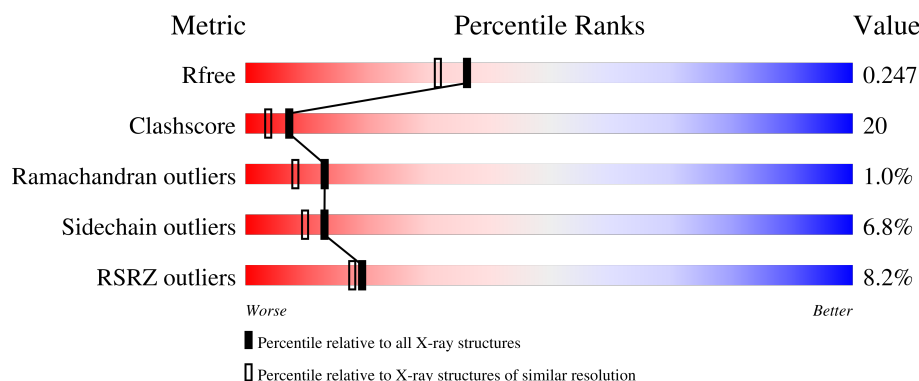
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	726	<div> <div>9%</div> <div>70%</div> <div>25%</div> <div>.</div> </div>
1	B	726	<div> <div>12%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>
1	C	726	<div> <div>6%</div> <div>66%</div> <div>30%</div> <div>.</div> </div>
1	D	726	<div> <div>6%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>

2 Entry composition [i](#)

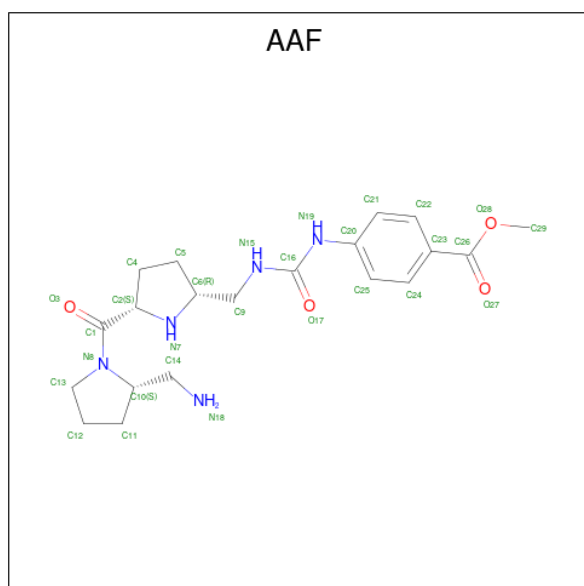
There are 3 unique types of molecules in this entry. The entry contains 28111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	B	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	C	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	D	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			

- Molecule 2 is METHYL 4-{[({[(2R,5S)-5-{{[(2S)-2-(AMINOMETHYL)PYRROLIDIN-1-YL] CARBONYL}PYRROLIDIN-2-YL]METHYL}AMINO)CARBONYL]AMINO}BENZOATE (three-letter code: AAF) (formula: C₂₀H₂₉N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	20	5	4		

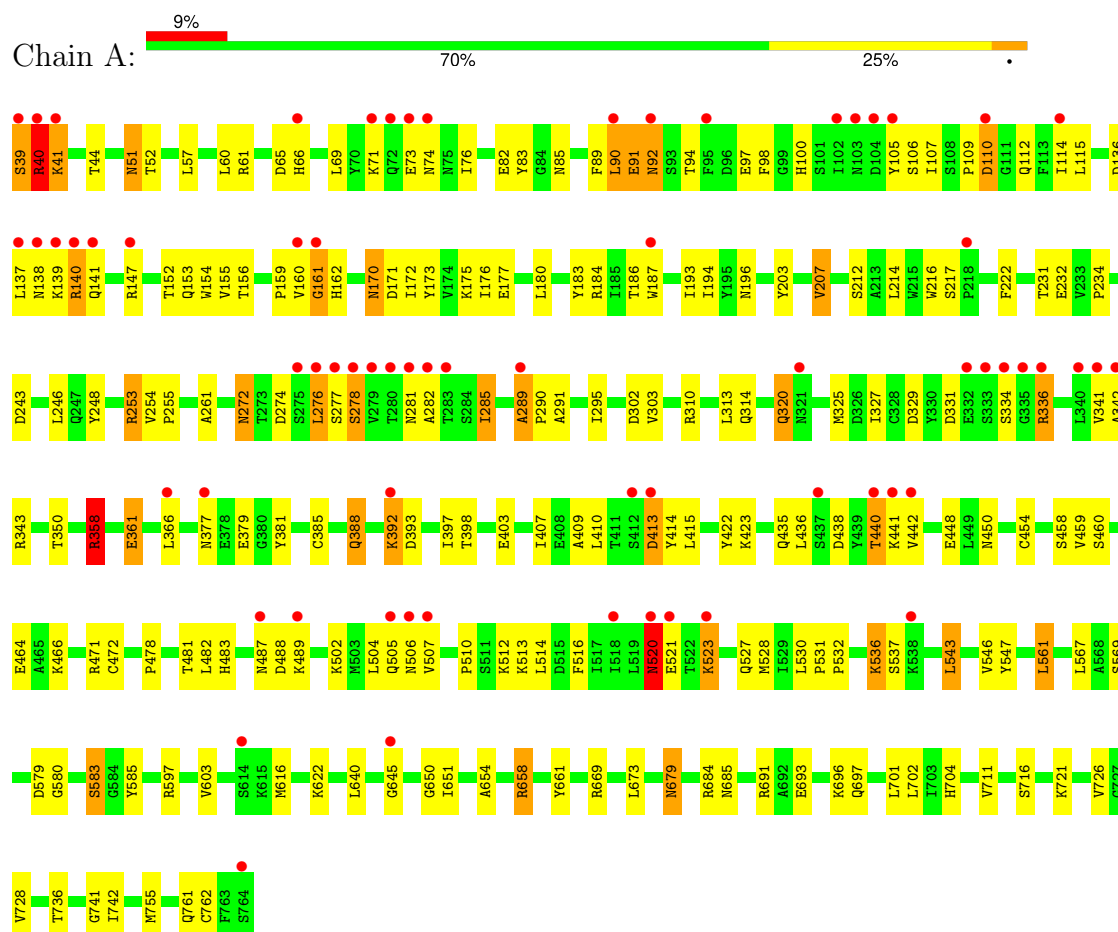
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1195	Total 1195	O 1195	0	0
3	B	1121	Total 1121	O 1121	0	0
3	C	938	Total 938	O 938	0	0
3	D	1032	Total 1032	O 1032	0	0

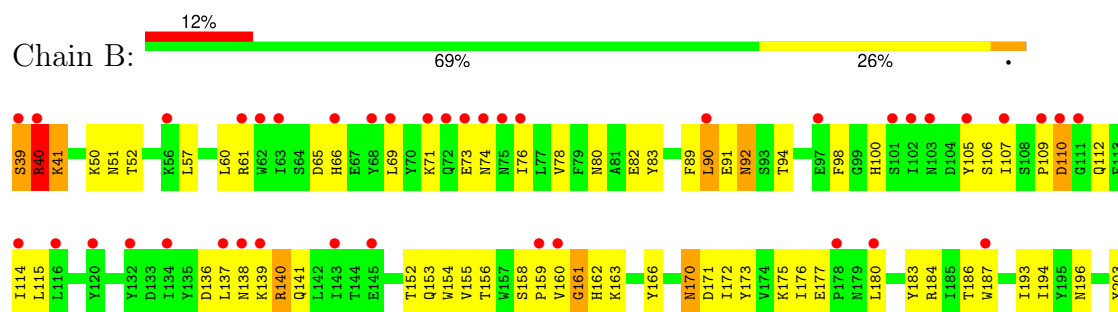
3 Residue-property plots

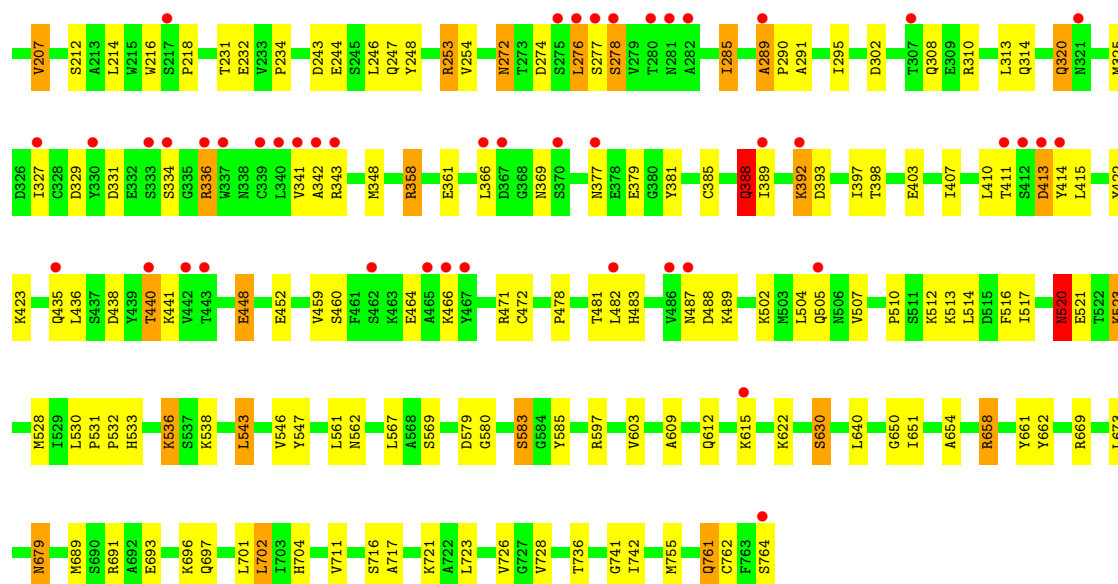
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dipeptidyl peptidase 4

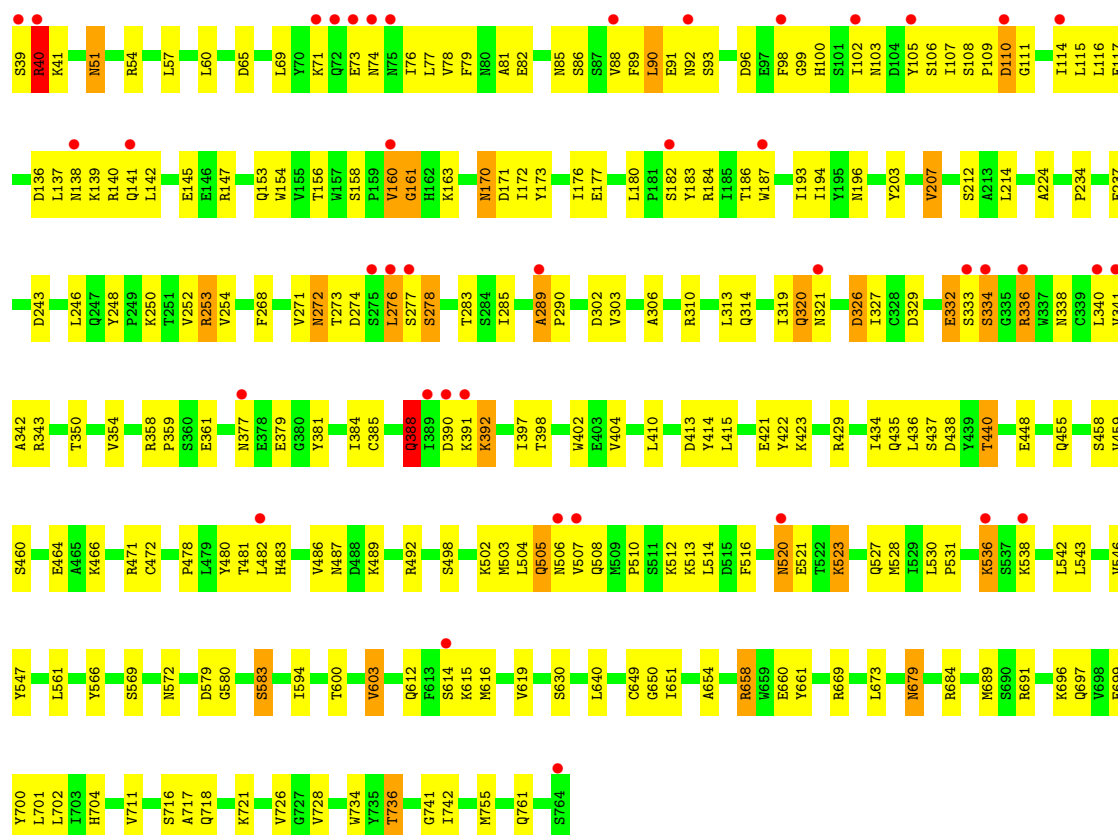


• Molecule 1: Dipeptidyl peptidase 4



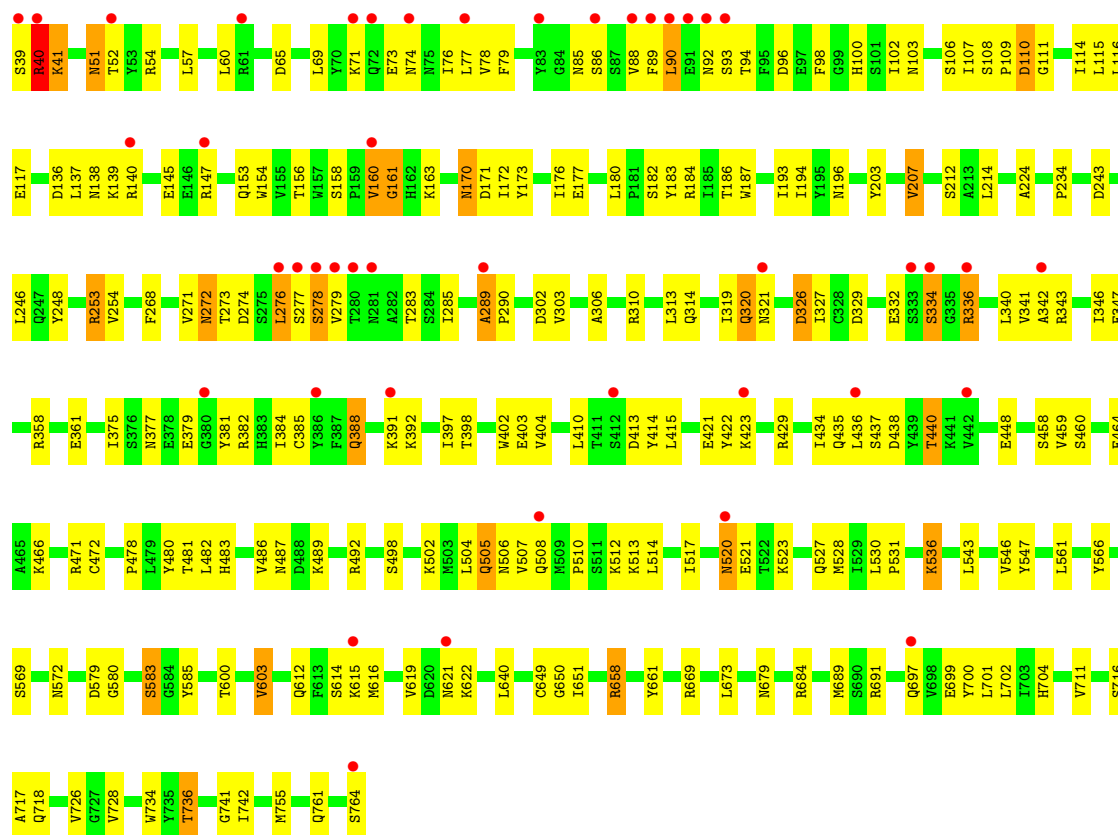


• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.13Å 126.50Å 127.37Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.7 (20.00-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.251 0.210 , 0.247	Depositor DCC
R_{free} test set	12847 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28111	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/6120	0.67	4/8321 (0.0%)
1	B	0.36	1/6120 (0.0%)	0.71	4/8321 (0.0%)
1	C	0.32	0/6120	0.62	1/8321 (0.0%)
1	D	0.33	0/6120	0.62	1/8321 (0.0%)
All	All	0.34	1/24480 (0.0%)	0.66	10/33284 (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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	630	SER	C-O	7.92	1.38	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ARG	NE-CZ-NH2	18.50	129.55	120.30
1	B	358	ARG	NE-CZ-NH1	-17.66	111.47	120.30
1	A	358	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	358	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	358	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	358	ARG	CD-NE-CZ	5.98	131.97	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	GLN	N-CA-C	-5.54	96.03	111.00
1	B	388	GLN	N-CA-C	-5.36	96.52	111.00
1	D	388	GLN	N-CA-C	-5.13	97.15	111.00
1	C	388	GLN	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	700	TYR	Sidechain
1	D	700	TYR	Sidechain

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	5949	0	5667	236	0
1	B	5949	0	5666	233	0
1	C	5949	0	5667	253	0
1	D	5949	0	5667	243	0
2	B	29	0	27	1	0
3	A	1195	0	0	63	0
3	B	1121	0	0	59	0
3	C	938	0	0	72	0
3	D	1032	0	0	67	0
All	All	28111	0	22694	949	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (949) 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:A:736:THR:HB	3:B:1870:HOH:O	1.37	1.24
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.25	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.28	1.12
1:A:736:THR:HG21	1:B:721:LYS:HB2	1.31	1.06
1:C:114:ILE:HD11	1:C:137:LEU:HD21	1.37	1.06
1:D:114:ILE:HD11	1:D:137:LEU:HD21	1.37	1.05
1:D:289:ALA:HB1	1:D:290:PRO:HA	1.35	1.04
1:A:721:LYS:HB2	1:B:736:THR:HG21	1.35	1.02
1:C:289:ALA:HB1	1:C:290:PRO:HA	1.36	1.01
1:C:176:ILE:HD11	1:C:276:LEU:HD21	1.43	0.99
1:D:176:ILE:HD11	1:D:276:LEU:HD21	1.43	0.98
1:D:621:ASN:HB3	3:D:768:HOH:O	1.66	0.96
1:D:528:MET:HE3	1:D:530:LEU:HD21	1.49	0.95
1:C:528:MET:HE3	1:C:530:LEU:HD21	1.50	0.93
1:A:289:ALA:HB1	1:A:290:PRO:CA	1.99	0.93
1:A:736:THR:CG2	1:B:721:LYS:HB2	2.03	0.89
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.02	0.88
1:A:736:THR:HG22	3:B:802:HOH:O	1.75	0.87
1:D:40:ARG:HA	3:D:854:HOH:O	1.73	0.87
1:D:76:ILE:HD12	1:D:90:LEU:HD11	1.57	0.86
1:B:334:SER:HB3	1:B:336:ARG:NE	1.91	0.86
1:B:615:LYS:HE3	3:B:1586:HOH:O	1.76	0.86
1:D:361:GLU:HG2	3:D:933:HOH:O	1.74	0.85
1:A:310:ARG:HH12	1:A:343:ARG:NH1	1.75	0.85
1:A:334:SER:HB3	1:A:336:ARG:NE	1.92	0.85
1:D:89:PHE:HD1	1:D:90:LEU:HD12	1.42	0.85
1:C:76:ILE:HG22	3:C:1495:HOH:O	1.76	0.85
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.57	0.84
1:A:721:LYS:HB2	1:B:736:THR:CG2	2.06	0.84
1:B:160:VAL:HG23	1:B:161:GLY:H	1.43	0.84
1:A:334:SER:HB3	1:A:336:ARG:HE	1.43	0.83
1:A:487:ASN:HB2	3:A:788:HOH:O	1.77	0.83
1:A:762:CYS:HB2	3:A:1511:HOH:O	1.78	0.83
1:A:172:ILE:H	1:A:186:THR:HG22	1.43	0.83
1:B:172:ILE:H	1:B:186:THR:HG22	1.43	0.82
1:B:334:SER:HB3	1:B:336:ARG:HE	1.42	0.82
1:C:276:LEU:HD22	1:C:276:LEU:H	1.45	0.82
1:A:289:ALA:HB2	3:A:1489:HOH:O	1.80	0.81
1:D:276:LEU:H	1:D:276:LEU:HD22	1.43	0.81
1:A:253:ARG:HH22	1:B:253:ARG:HH22	1.25	0.81
1:B:310:ARG:HH12	1:B:343:ARG:NH1	1.79	0.81
1:B:702:LEU:HD22	3:B:1886:HOH:O	1.80	0.81
1:C:89:PHE:HD1	1:C:90:LEU:HD12	1.42	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:H	1:C:186:THR:HG22	1.46	0.80
1:C:528:MET:CE	1:C:530:LEU:HD21	2.12	0.80
1:B:140:ARG:HH11	1:B:140:ARG:HG2	1.48	0.79
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.48	0.79
1:A:160:VAL:HG23	1:A:161:GLY:H	1.45	0.79
1:D:172:ILE:H	1:D:186:THR:HG22	1.46	0.79
1:B:276:LEU:HB3	3:B:1234:HOH:O	1.82	0.79
1:A:341:VAL:O	1:A:342:ALA:HB3	1.82	0.79
1:D:528:MET:CE	1:D:530:LEU:HD21	2.13	0.78
1:B:207:VAL:O	1:B:358:ARG:NH2	2.16	0.78
1:A:358:ARG:NH1	3:A:1447:HOH:O	2.17	0.78
1:A:281:ASN:HB2	3:A:1179:HOH:O	1.84	0.78
1:B:448:GLU:HG3	3:B:1613:HOH:O	1.84	0.78
1:D:726:VAL:HG12	1:D:728:VAL:HG23	1.66	0.77
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.67	0.77
1:C:334:SER:HB3	1:C:336:ARG:HE	1.48	0.77
1:D:334:SER:HB3	1:D:336:ARG:HE	1.48	0.77
1:B:176:ILE:HD11	1:B:276:LEU:HD21	1.66	0.77
1:C:726:VAL:HG12	1:C:728:VAL:HG23	1.66	0.77
1:A:255:PRO:HD2	3:A:1931:HOH:O	1.83	0.77
1:A:289:ALA:CB	1:A:290:PRO:HA	2.12	0.76
1:A:282:ALA:HB3	3:A:1913:HOH:O	1.84	0.76
1:A:489:LYS:NZ	1:A:489:LYS:HB3	2.01	0.76
1:B:528:MET:HE3	1:B:530:LEU:HD21	1.68	0.76
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.67	0.76
1:B:341:VAL:HB	3:B:887:HOH:O	1.86	0.75
1:C:717:ALA:O	1:D:736:THR:HG21	1.86	0.75
1:A:505:GLN:HB3	3:A:1559:HOH:O	1.85	0.75
1:A:52:THR:HG22	3:A:1873:HOH:O	1.85	0.75
1:D:289:ALA:HB1	1:D:290:PRO:CA	2.15	0.75
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.69	0.75
1:B:489:LYS:NZ	1:B:489:LYS:HB3	2.00	0.75
1:B:517:ILE:HD13	3:B:1143:HOH:O	1.87	0.75
1:B:289:ALA:CB	1:B:290:PRO:HA	2.15	0.74
1:B:723:LEU:HA	3:B:1900:HOH:O	1.86	0.74
1:A:438:ASP:OD1	1:A:440:THR:HB	1.87	0.74
1:C:90:LEU:O	1:C:90:LEU:HD22	1.86	0.74
1:C:736:THR:HG21	1:D:717:ALA:O	1.88	0.74
1:C:289:ALA:HB1	1:C:290:PRO:CA	2.16	0.74
1:D:90:LEU:HD22	1:D:90:LEU:O	1.87	0.74
1:B:528:MET:CE	1:B:530:LEU:HD21	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:HE1	1:C:277:SER:O	1.71	0.74
1:B:184:ARG:HD3	1:B:186:THR:O	1.88	0.74
1:B:327:ILE:HB	1:B:343:ARG:HG2	1.69	0.74
1:C:276:LEU:HB3	3:C:1068:HOH:O	1.88	0.73
1:D:614:SER:HB2	3:D:768:HOH:O	1.88	0.73
1:D:289:ALA:HB2	3:D:1585:HOH:O	1.88	0.73
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.88	0.73
1:C:272:ASN:ND2	1:C:274:ASP:H	1.86	0.73
1:A:350:THR:HG23	3:A:1787:HOH:O	1.89	0.73
1:D:272:ASN:ND2	1:D:274:ASP:H	1.87	0.73
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.70	0.73
1:C:594:ILE:HG13	3:C:1263:HOH:O	1.89	0.72
1:A:622:LYS:HE3	3:A:1560:HOH:O	1.88	0.72
1:B:171:ASP:OD1	1:B:186:THR:HG23	1.90	0.72
1:A:528:MET:CE	1:A:530:LEU:HD21	2.19	0.72
1:A:184:ARG:HD3	1:A:186:THR:O	1.89	0.72
1:C:684:ARG:HD3	3:C:1582:HOH:O	1.89	0.72
1:A:207:VAL:O	1:A:358:ARG:NH2	2.23	0.71
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.91	0.71
1:D:684:ARG:HG3	3:D:1162:HOH:O	1.89	0.71
1:C:361:GLU:HG2	3:C:955:HOH:O	1.89	0.71
1:B:438:ASP:OD1	1:B:440:THR:HB	1.90	0.71
1:D:183:TYR:HE1	1:D:277:SER:O	1.73	0.71
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.26	0.70
1:D:673:LEU:HG	3:D:1710:HOH:O	1.89	0.70
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.26	0.70
1:C:142:LEU:HG	3:C:1702:HOH:O	1.89	0.70
1:D:334:SER:HB3	1:D:336:ARG:NE	2.07	0.70
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.72	0.70
1:C:334:SER:HB3	1:C:336:ARG:NE	2.07	0.70
1:B:341:VAL:O	1:B:342:ALA:HB3	1.90	0.70
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.40	0.70
1:D:177:GLU:HB2	1:D:180:LEU:HD22	1.72	0.70
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.92	0.70
1:C:359:PRO:HA	3:C:1500:HOH:O	1.92	0.70
1:D:600:THR:O	1:D:603:VAL:HG13	1.92	0.70
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.90	0.69
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.74	0.69
1:D:379:GLU:HB2	3:D:1305:HOH:O	1.91	0.69
1:B:597:ARG:HH12	1:B:679:ASN:HD21	1.40	0.69
1:B:704:HIS:HB2	3:B:1886:HOH:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HD3	1:D:186:THR:O	1.92	0.69
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.90	0.69
1:A:392:LYS:HG3	3:A:1107:HOH:O	1.91	0.69
1:B:471:ARG:HB3	3:B:1550:HOH:O	1.92	0.69
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.75	0.68
1:C:103:ASN:HB2	3:C:1205:HOH:O	1.92	0.68
1:C:600:THR:O	1:C:603:VAL:HG13	1.93	0.68
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.94	0.68
1:D:347:GLU:HG3	3:D:1766:HOH:O	1.94	0.68
1:A:51:ASN:HB2	3:A:972:HOH:O	1.93	0.68
1:A:97:GLU:HB3	3:A:1936:HOH:O	1.93	0.68
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.76	0.68
3:A:771:HOH:O	1:B:736:THR:HG22	1.92	0.68
1:C:184:ARG:HD3	1:C:186:THR:O	1.94	0.68
1:C:358:ARG:HD2	3:C:1669:HOH:O	1.93	0.68
1:A:90:LEU:O	1:A:90:LEU:HD13	1.94	0.67
1:A:253:ARG:HD3	3:A:1922:HOH:O	1.93	0.67
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.94	0.67
1:C:109:PRO:HB2	1:C:160:VAL:O	1.94	0.67
1:D:109:PRO:HB2	1:D:160:VAL:O	1.93	0.67
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.75	0.67
1:A:450:ASN:HB3	3:A:1607:HOH:O	1.94	0.67
1:B:90:LEU:HD13	1:B:90:LEU:O	1.95	0.67
1:C:98:PHE:HA	3:C:1652:HOH:O	1.93	0.67
1:A:74:ASN:C	1:A:92:ASN:HB3	2.15	0.67
1:A:310:ARG:NE	3:A:1515:HOH:O	2.26	0.67
1:B:74:ASN:C	1:B:92:ASN:HB3	2.15	0.67
1:C:203:TYR:HA	1:C:207:VAL:CG1	2.25	0.67
1:C:82:GLU:HG2	3:C:1535:HOH:O	1.94	0.66
1:D:203:TYR:HA	1:D:207:VAL:CG1	2.25	0.66
1:D:203:TYR:CD2	1:D:207:VAL:HG11	2.29	0.66
1:D:69:LEU:CD1	1:D:107:ILE:HD12	2.25	0.66
1:C:203:TYR:CD2	1:C:207:VAL:HG11	2.30	0.66
1:C:69:LEU:CD1	1:C:107:ILE:HD12	2.25	0.66
1:B:272:ASN:ND2	1:B:274:ASP:H	1.94	0.66
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.78	0.66
1:B:379:GLU:HB2	3:B:1743:HOH:O	1.94	0.66
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.78	0.66
1:D:171:ASP:OD1	1:D:186:THR:HG23	1.96	0.66
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.78	0.66
1:B:52:THR:HB	3:B:1656:HOH:O	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HG2	3:C:1268:HOH:O	1.95	0.65
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.77	0.65
1:B:109:PRO:HB2	1:B:160:VAL:O	1.96	0.65
1:D:276:LEU:H	1:D:276:LEU:CD2	2.10	0.65
1:A:272:ASN:ND2	1:A:274:ASP:H	1.95	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.95	0.65
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.78	0.64
1:D:580:GLY:O	1:D:583:SER:HB2	1.97	0.64
1:C:171:ASP:OD1	1:C:186:THR:HG23	1.97	0.64
1:C:489:LYS:NZ	1:C:489:LYS:HB3	2.13	0.64
1:D:489:LYS:NZ	1:D:489:LYS:HB3	2.12	0.64
1:A:160:VAL:HG23	1:A:161:GLY:N	2.13	0.64
1:C:361:GLU:HG2	3:C:1108:HOH:O	1.97	0.64
1:D:279:VAL:HB	3:D:1273:HOH:O	1.97	0.64
1:B:65:ASP:OD2	1:B:466:LYS:HB2	1.98	0.64
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.63	0.64
1:A:41:LYS:HB2	3:A:1293:HOH:O	1.98	0.64
1:A:697:GLN:HG3	3:A:1278:HOH:O	1.97	0.64
1:C:51:ASN:HB2	3:C:1687:HOH:O	1.98	0.63
1:A:109:PRO:HB2	1:A:160:VAL:O	1.99	0.63
1:A:276:LEU:CD2	1:A:276:LEU:H	2.12	0.63
1:B:762:CYS:HB2	3:B:1418:HOH:O	1.98	0.63
1:C:319:ILE:HG13	3:C:1697:HOH:O	1.98	0.63
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.99	0.63
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.96	0.63
1:A:693:GLU:OE1	1:A:696:LYS:HE2	1.97	0.63
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.34	0.63
1:B:693:GLU:OE1	1:B:696:LYS:HE2	1.98	0.63
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.34	0.63
1:B:160:VAL:HG23	1:B:161:GLY:N	2.12	0.63
1:B:276:LEU:CD2	1:B:276:LEU:H	2.12	0.63
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.33	0.62
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.81	0.62
1:C:580:GLY:O	1:C:583:SER:HB2	1.99	0.62
1:C:684:ARG:HD2	3:C:1685:HOH:O	2.00	0.62
1:D:71:LYS:HB3	3:D:1461:HOH:O	1.98	0.62
1:B:243:ASP:HB3	3:B:1378:HOH:O	1.99	0.62
1:B:272:ASN:HD22	1:B:274:ASP:H	1.46	0.62
1:D:341:VAL:O	1:D:342:ALA:HB3	2.00	0.62
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.30	0.62
1:C:272:ASN:HD22	1:C:274:ASP:H	1.47	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:PRO:HG3	1:C:326:ASP:OD2	2.00	0.62
1:D:486:VAL:HG13	1:D:487:ASN:N	2.15	0.61
1:D:54:ARG:HG2	3:D:1295:HOH:O	2.01	0.61
1:D:346:ILE:HG13	3:D:1329:HOH:O	1.99	0.61
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.65	0.61
1:D:410:LEU:HD13	1:D:415:LEU:HD23	1.82	0.61
1:B:483:HIS:HD2	3:B:921:HOH:O	1.83	0.61
1:C:390:ASP:HB3	3:C:857:HOH:O	1.99	0.61
1:D:52:THR:HG21	3:D:1570:HOH:O	1.99	0.61
1:C:114:ILE:CD1	1:C:137:LEU:HD21	2.24	0.61
1:C:486:VAL:HG13	1:C:487:ASN:N	2.16	0.61
1:B:277:SER:O	1:B:278:SER:HB3	2.00	0.61
1:C:341:VAL:O	1:C:342:ALA:HB3	2.01	0.61
1:A:277:SER:O	1:A:278:SER:HB3	2.00	0.61
1:A:272:ASN:HD22	1:A:274:ASP:H	1.49	0.60
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.31	0.60
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.83	0.60
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.83	0.60
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.30	0.60
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.83	0.60
1:D:114:ILE:CD1	1:D:137:LEU:HD21	2.23	0.60
1:B:489:LYS:HB3	1:B:489:LYS:HZ3	1.66	0.60
1:A:366:LEU:HD23	3:A:1245:HOH:O	2.00	0.60
1:C:77:LEU:HD23	1:C:88:VAL:HA	1.84	0.60
1:C:276:LEU:H	1:C:276:LEU:CD2	2.11	0.60
1:D:77:LEU:HD23	1:D:88:VAL:HA	1.84	0.60
1:A:377:ASN:HB2	1:A:381:TYR:O	2.02	0.60
1:C:614:SER:HA	1:C:619:VAL:HB	1.84	0.60
1:D:614:SER:HA	1:D:619:VAL:HB	1.83	0.60
1:C:272:ASN:HD22	1:C:272:ASN:C	2.05	0.60
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.01	0.60
1:D:76:ILE:HB	1:D:90:LEU:CD1	2.31	0.60
1:B:471:ARG:HD2	3:B:1711:HOH:O	2.02	0.60
1:D:140:ARG:HG2	1:D:140:ARG:HH11	1.66	0.60
1:D:272:ASN:HD22	1:D:272:ASN:C	2.05	0.60
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.84	0.60
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.67	0.59
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.83	0.59
1:C:65:ASP:OD2	1:C:466:LYS:HB2	2.02	0.59
1:D:182:SER:HB3	3:D:1765:HOH:O	2.03	0.59
1:A:261:ALA:HB2	3:B:1915:HOH:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LYS:HD3	3:B:1081:HOH:O	2.01	0.59
1:D:93:SER:HB2	1:D:96:ASP:OD2	2.02	0.59
1:D:336:ARG:HB3	3:D:1546:HOH:O	2.03	0.59
1:B:691:ARG:NE	3:B:1749:HOH:O	2.18	0.59
1:B:114:ILE:CD1	1:B:137:LEU:HD21	2.32	0.59
1:B:612:GLN:HB2	3:B:1143:HOH:O	2.03	0.59
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.31	0.59
1:B:289:ALA:HB2	3:B:1085:HOH:O	2.02	0.59
1:B:377:ASN:HB2	1:B:381:TYR:O	2.02	0.59
1:B:693:GLU:HA	1:B:726:VAL:HG11	1.85	0.59
1:C:93:SER:HB2	1:C:96:ASP:OD2	2.02	0.59
1:C:651:ILE:HG21	1:C:755:MET:HE2	1.85	0.59
1:C:721:LYS:HG2	3:C:1313:HOH:O	2.01	0.59
1:C:513:LYS:HD2	3:C:1508:HOH:O	2.03	0.59
1:D:65:ASP:OD2	1:D:466:LYS:HB2	2.02	0.59
1:A:139:LYS:HD3	3:A:1411:HOH:O	2.02	0.58
1:D:342:ALA:HA	3:D:1699:HOH:O	2.02	0.58
1:A:89:PHE:CE1	1:A:107:ILE:HD13	2.38	0.58
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.38	0.58
1:A:71:LYS:HG2	1:A:76:ILE:HG12	1.85	0.58
1:B:348:MET:HG3	3:B:1665:HOH:O	2.03	0.58
1:C:194:ILE:HD12	3:C:1007:HOH:O	2.02	0.58
1:C:338:ASN:HB2	3:C:1328:HOH:O	2.03	0.58
1:A:334:SER:CB	1:A:336:ARG:HE	2.15	0.58
1:A:651:ILE:HG21	1:A:755:MET:CE	2.34	0.58
1:D:272:ASN:HD22	1:D:274:ASP:H	1.48	0.58
1:A:506:ASN:HB2	3:A:1502:HOH:O	2.03	0.58
1:B:172:ILE:H	1:B:186:THR:CG2	2.13	0.58
1:B:248:TYR:HE1	3:B:1915:HOH:O	1.85	0.58
1:C:103:ASN:OD1	1:C:117:GLU:HG2	2.03	0.58
1:D:194:ILE:HD12	3:D:1007:HOH:O	2.03	0.58
1:D:193:ILE:HG22	1:D:194:ILE:HG13	1.85	0.58
1:B:523:LYS:HG2	3:B:1411:HOH:O	2.04	0.58
1:C:172:ILE:HB	3:C:1474:HOH:O	2.03	0.58
1:D:41:LYS:HD2	3:D:1713:HOH:O	2.02	0.58
1:A:341:VAL:O	1:A:342:ALA:CB	2.47	0.58
1:B:71:LYS:HG2	1:B:76:ILE:HG12	1.86	0.58
1:B:334:SER:CB	1:B:336:ARG:HE	2.14	0.58
1:B:452:GLU:HG2	3:B:1827:HOH:O	2.03	0.58
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.39	0.58
1:D:327:ILE:HB	1:D:343:ARG:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.86	0.57
1:C:422:TYR:CE2	1:C:423:LYS:HD3	2.39	0.57
1:D:621:ASN:HB3	3:D:1531:HOH:O	2.03	0.57
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.40	0.57
1:B:651:ILE:HG21	1:B:755:MET:CE	2.34	0.57
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.86	0.57
1:C:203:TYR:HA	1:C:207:VAL:HG12	1.86	0.57
1:A:172:ILE:H	1:A:186:THR:CG2	2.15	0.57
1:D:41:LYS:HB2	3:D:1768:HOH:O	2.04	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:D:651:ILE:CD1	1:D:755:MET:HE2	2.34	0.57
1:A:684:ARG:HD2	3:A:1478:HOH:O	2.05	0.57
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.85	0.57
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.85	0.57
1:A:243:ASP:HB3	3:A:1428:HOH:O	2.05	0.57
1:A:44:THR:HB	3:A:1011:HOH:O	2.04	0.57
1:B:232:GLU:HG2	3:B:1795:HOH:O	2.05	0.57
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.85	0.56
1:A:489:LYS:HB3	1:A:489:LYS:HZ3	1.70	0.56
1:D:103:ASN:OD1	1:D:117:GLU:HG2	2.04	0.56
1:A:71:LYS:HB3	3:A:1376:HOH:O	2.05	0.56
1:C:156:THR:HG21	1:C:214:LEU:HD11	1.87	0.56
1:A:651:ILE:HD13	1:A:755:MET:HE2	1.87	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.87	0.56
1:B:651:ILE:CD1	1:B:755:MET:HE2	2.35	0.56
1:C:69:LEU:HD22	3:C:1495:HOH:O	2.03	0.56
1:C:704:HIS:HD2	1:C:716:SER:OG	1.88	0.56
1:D:651:ILE:HG21	1:D:755:MET:CE	2.34	0.56
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.87	0.56
1:C:327:ILE:HB	1:C:343:ARG:HG2	1.86	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.85	0.56
1:D:277:SER:O	1:D:278:SER:HB3	2.05	0.56
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.25	0.56
1:C:651:ILE:HG21	1:C:755:MET:CE	2.36	0.56
1:B:538:LYS:HG2	3:B:1442:HOH:O	2.06	0.56
1:D:512:LYS:HD3	3:D:1446:HOH:O	2.06	0.56
1:D:622:LYS:HE3	3:D:1439:HOH:O	2.06	0.56
1:A:272:ASN:HD22	1:A:272:ASN:C	2.10	0.56
1:D:203:TYR:HA	1:D:207:VAL:HG12	1.87	0.56
1:D:156:THR:HG21	1:D:214:LEU:HD11	1.87	0.55
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.26	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HD2	1:C:508:GLN:HG3	1.88	0.55
1:C:69:LEU:HD13	1:C:107:ILE:HD12	1.88	0.55
1:C:183:TYR:CE1	1:C:277:SER:O	2.58	0.55
1:C:71:LYS:HE2	3:C:1293:HOH:O	2.06	0.55
1:A:276:LEU:HB3	3:A:1157:HOH:O	2.06	0.55
1:B:487:ASN:HB2	3:B:1750:HOH:O	2.05	0.55
1:D:69:LEU:HD13	1:D:107:ILE:HD12	1.88	0.55
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.89	0.55
1:A:651:ILE:CD1	1:A:755:MET:HE2	2.37	0.55
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.55
1:C:340:LEU:O	1:C:343:ARG:HB3	2.07	0.55
1:D:183:TYR:CD2	1:D:276:LEU:HG	2.41	0.55
1:D:278:SER:HA	3:D:1433:HOH:O	2.06	0.55
1:D:342:ALA:HB1	3:D:1637:HOH:O	2.07	0.55
1:A:170:ASN:N	1:A:170:ASN:HD22	2.04	0.55
1:A:435:GLN:NE2	1:A:441:LYS:CD	2.70	0.55
1:C:277:SER:O	1:C:278:SER:HB3	2.06	0.55
1:A:413:ASP:HB2	3:A:1527:HOH:O	2.05	0.55
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.90	0.55
1:D:651:ILE:HD13	1:D:755:MET:HE2	1.88	0.54
1:B:413:ASP:HB2	3:B:1889:HOH:O	2.07	0.54
1:D:379:GLU:HG2	3:D:1512:HOH:O	2.06	0.54
1:D:726:VAL:CG1	1:D:728:VAL:HG23	2.37	0.54
1:D:40:ARG:HD2	1:D:508:GLN:HG3	1.88	0.54
1:D:71:LYS:HE2	3:D:1440:HOH:O	2.06	0.54
1:A:281:ASN:ND2	3:A:1642:HOH:O	2.39	0.54
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.89	0.54
1:B:114:ILE:HD12	1:B:137:LEU:HD21	1.89	0.54
1:B:651:ILE:HD13	1:B:755:MET:HE2	1.88	0.54
1:C:183:TYR:CD2	1:C:276:LEU:HG	2.41	0.54
1:C:579:ASP:HB3	1:C:583:SER:OG	2.07	0.54
1:D:170:ASN:N	1:D:170:ASN:HD22	2.06	0.54
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.42	0.54
1:B:170:ASN:N	1:B:170:ASN:HD22	2.06	0.54
1:D:651:ILE:HG21	1:D:755:MET:HE2	1.89	0.54
1:A:658:ARG:NH2	1:B:244:GLU:OE2	2.40	0.54
1:B:183:TYR:HE1	1:B:277:SER:O	1.91	0.54
1:B:272:ASN:HD22	1:B:272:ASN:C	2.10	0.54
1:B:704:HIS:HD2	1:B:716:SER:OG	1.91	0.54
1:C:57:LEU:HD21	3:C:1553:HOH:O	2.08	0.54
1:A:459:VAL:HG22	1:A:460:SER:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:CB	1:B:290:PRO:CA	2.78	0.54
1:C:651:ILE:CD1	1:C:755:MET:HE2	2.38	0.54
1:D:340:LEU:O	1:D:343:ARG:HB3	2.07	0.54
1:A:597:ARG:NH1	1:A:679:ASN:HD21	2.06	0.54
1:C:332:GLU:HB2	3:C:1548:HOH:O	2.07	0.54
1:D:289:ALA:CB	1:D:290:PRO:HA	2.24	0.53
1:D:615:LYS:NZ	3:D:1056:HOH:O	2.41	0.53
1:B:502:LYS:O	1:B:505:GLN:HG2	2.09	0.53
1:D:704:HIS:HD2	1:D:716:SER:OG	1.91	0.53
1:A:114:ILE:HD12	1:A:137:LEU:HD21	1.89	0.53
1:C:341:VAL:HG12	3:C:1320:HOH:O	2.07	0.53
1:A:379:GLU:HG3	3:A:1198:HOH:O	2.07	0.53
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.44	0.53
1:B:726:VAL:HB	3:B:1900:HOH:O	2.08	0.53
1:A:704:HIS:HD2	1:A:716:SER:OG	1.92	0.53
1:C:486:VAL:HG13	1:C:487:ASN:H	1.73	0.53
1:D:147:ARG:HB2	3:D:1010:HOH:O	2.09	0.53
1:C:243:ASP:HB3	3:C:1034:HOH:O	2.09	0.53
1:D:615:LYS:HG2	3:D:1056:HOH:O	2.08	0.53
1:B:90:LEU:C	1:B:90:LEU:HD22	2.28	0.53
1:A:658:ARG:HG3	1:A:658:ARG:O	2.08	0.53
1:B:389:ILE:HD13	3:B:1167:HOH:O	2.08	0.53
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.89	0.53
1:B:520:ASN:O	1:B:521:GLU:HB2	2.09	0.53
1:C:333:SER:HB2	3:C:1523:HOH:O	2.09	0.53
1:C:651:ILE:HD13	1:C:755:MET:HE2	1.91	0.53
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.91	0.52
1:A:90:LEU:C	1:A:90:LEU:HD22	2.30	0.52
1:C:342:ALA:HB3	3:C:1701:HOH:O	2.08	0.52
1:D:579:ASP:HB3	1:D:583:SER:OG	2.10	0.52
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.90	0.52
1:A:520:ASN:O	1:A:521:GLU:HB2	2.09	0.52
1:C:105:TYR:HB2	3:C:1293:HOH:O	2.09	0.52
1:D:486:VAL:HG13	1:D:487:ASN:H	1.73	0.52
1:A:622:LYS:HB2	1:A:622:LYS:NZ	2.25	0.52
1:A:736:THR:HG21	1:B:721:LYS:CB	2.22	0.52
1:C:736:THR:HG23	3:D:778:HOH:O	2.10	0.52
1:D:40:ARG:NH1	3:D:1185:HOH:O	2.42	0.52
1:D:377:ASN:HB3	1:D:379:GLU:H	1.73	0.52
1:A:502:LYS:O	1:A:505:GLN:HG2	2.09	0.52
1:B:471:ARG:HG3	3:B:1697:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HD3	1:C:507:VAL:C	2.30	0.52
1:A:183:TYR:HE1	1:A:277:SER:O	1.92	0.52
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.91	0.52
1:A:325:MET:HE2	1:A:327:ILE:HG12	1.92	0.52
1:C:89:PHE:CE1	1:C:107:ILE:HD13	2.45	0.52
1:D:76:ILE:HB	1:D:90:LEU:HD13	1.91	0.52
1:A:435:GLN:NE2	1:A:441:LYS:HD2	2.25	0.52
1:B:140:ARG:HG2	1:B:140:ARG:NH1	2.21	0.52
1:A:276:LEU:CD2	1:A:276:LEU:N	2.73	0.52
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.92	0.52
1:C:422:TYR:CD2	1:C:423:LYS:HD3	2.45	0.52
1:D:40:ARG:HD3	1:D:507:VAL:C	2.30	0.52
1:D:422:TYR:CE2	1:D:423:LYS:HD3	2.44	0.52
1:A:342:ALA:HB3	3:A:1804:HOH:O	2.08	0.51
1:A:379:GLU:HG2	1:A:381:TYR:CD1	2.45	0.51
1:D:536:LYS:HE2	3:D:1692:HOH:O	2.10	0.51
1:D:658:ARG:HG2	1:D:661:TYR:CE2	2.45	0.51
1:C:76:ILE:HB	1:C:90:LEU:HD13	1.91	0.51
1:C:99:GLY:HA3	3:C:1653:HOH:O	2.10	0.51
1:C:726:VAL:CG1	1:C:728:VAL:HG23	2.38	0.51
1:D:94:THR:HB	3:D:1445:HOH:O	2.09	0.51
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.92	0.51
1:D:472:CYS:O	1:D:478:PRO:HA	2.10	0.51
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.45	0.51
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.51
1:C:377:ASN:HB2	1:C:381:TYR:O	2.11	0.51
1:B:597:ARG:NH1	1:B:679:ASN:HD21	2.06	0.51
1:C:536:LYS:HE3	3:C:1111:HOH:O	2.11	0.51
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.91	0.51
1:D:183:TYR:CE1	1:D:277:SER:O	2.60	0.51
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.21	0.51
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.46	0.51
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.75	0.51
1:C:377:ASN:HB3	1:C:379:GLU:H	1.75	0.51
1:D:89:PHE:CE1	1:D:107:ILE:HD13	2.46	0.51
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.93	0.51
1:B:513:LYS:HE3	1:B:530:LEU:HD11	1.93	0.51
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.32	0.51
1:D:277:SER:HA	3:D:1719:HOH:O	2.10	0.51
1:A:285:ILE:N	1:A:285:ILE:CD1	2.74	0.50
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:SER:O	1:C:40:ARG:O	2.29	0.50
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.93	0.50
1:A:392:LYS:HB3	3:A:1916:HOH:O	2.11	0.50
1:D:321:ASN:OD1	3:D:1754:HOH:O	2.19	0.50
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.92	0.50
1:B:41:LYS:HG3	3:B:986:HOH:O	2.12	0.50
1:D:40:ARG:HH11	1:D:40:ARG:CG	2.25	0.50
1:A:139:LYS:HD2	3:A:1532:HOH:O	2.12	0.50
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.76	0.50
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.45	0.50
1:D:435:GLN:OE1	1:D:437:SER:HB2	2.11	0.50
1:A:645:GLY:HA2	3:A:1050:HOH:O	2.11	0.50
1:C:489:LYS:HB3	1:C:489:LYS:HZ3	1.76	0.50
1:C:673:LEU:N	1:C:673:LEU:HD12	2.27	0.50
1:B:435:GLN:NE2	1:B:441:LYS:CD	2.74	0.50
1:B:459:VAL:HG22	1:B:460:SER:N	2.26	0.50
1:C:57:LEU:HD23	3:C:1025:HOH:O	2.11	0.50
1:C:472:CYS:O	1:C:478:PRO:HA	2.11	0.50
1:C:71:LYS:N	3:C:1251:HOH:O	2.44	0.50
1:B:741:GLY:O	1:B:742:ILE:C	2.50	0.50
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.93	0.50
1:C:612:GLN:O	1:C:616:MET:HG3	2.12	0.50
1:D:673:LEU:HD12	1:D:673:LEU:N	2.27	0.50
1:A:361:GLU:CD	3:A:1015:HOH:O	2.50	0.50
1:B:622:LYS:NZ	3:B:1303:HOH:O	2.44	0.50
1:C:136:ASP:OD1	1:C:138:ASN:HB2	2.12	0.50
1:C:438:ASP:OD1	1:C:440:THR:HB	2.12	0.50
1:D:74:ASN:C	1:D:92:ASN:HB3	2.32	0.50
1:D:612:GLN:O	1:D:616:MET:HG3	2.12	0.50
1:D:521:GLU:HA	3:D:1395:HOH:O	2.10	0.49
1:A:285:ILE:N	1:A:285:ILE:HD13	2.27	0.49
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.47	0.49
1:B:658:ARG:O	1:B:658:ARG:HG3	2.12	0.49
1:D:306:ALA:CB	1:D:310:ARG:HD2	2.42	0.49
1:D:438:ASP:OD1	1:D:440:THR:HB	2.12	0.49
1:B:285:ILE:CD1	1:B:285:ILE:N	2.75	0.49
1:B:291:ALA:O	1:B:295:ILE:HG23	2.13	0.49
1:C:186:THR:HB	3:C:1474:HOH:O	2.12	0.49
1:C:278:SER:N	3:C:1462:HOH:O	2.45	0.49
1:D:136:ASP:OD1	1:D:138:ASN:HB2	2.11	0.49
1:B:622:LYS:NZ	1:B:622:LYS:HB2	2.27	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:VAL:HG23	1:C:161:GLY:H	1.78	0.49
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.94	0.49
1:A:379:GLU:HB2	3:A:1810:HOH:O	2.11	0.49
1:A:513:LYS:HE3	1:A:530:LEU:HD11	1.94	0.49
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.94	0.49
1:C:306:ALA:CB	1:C:310:ARG:HD2	2.43	0.49
1:B:341:VAL:O	1:B:342:ALA:CB	2.56	0.49
1:B:392:LYS:HD2	1:B:393:ASP:N	2.28	0.49
1:C:314:GLN:HG3	3:C:946:HOH:O	2.13	0.49
1:B:71:LYS:NZ	1:B:105:TYR:HB2	2.28	0.49
1:B:379:GLU:HG2	1:B:381:TYR:CD1	2.47	0.49
1:C:504:LEU:HA	1:C:507:VAL:HG12	1.95	0.49
1:D:173:TYR:HB3	1:D:182:SER:OG	2.13	0.49
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.96	0.49
1:A:277:SER:O	1:A:278:SER:CB	2.61	0.49
1:C:74:ASN:C	1:C:92:ASN:HB3	2.33	0.49
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.94	0.49
1:D:276:LEU:HD23	1:D:276:LEU:O	2.12	0.49
1:D:718:GLN:HA	1:D:718:GLN:HE21	1.78	0.49
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.45	0.49
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.49
1:C:413:ASP:HB3	1:C:414:TYR:CD1	2.48	0.49
1:C:435:GLN:OE1	1:C:437:SER:HB2	2.11	0.49
1:C:139:LYS:HD3	3:C:1349:HOH:O	2.12	0.48
1:D:39:SER:O	1:D:40:ARG:O	2.31	0.48
1:D:140:ARG:HG2	1:D:140:ARG:NH1	2.27	0.48
1:D:697:GLN:HG3	3:D:1792:HOH:O	2.11	0.48
1:A:147:ARG:HG2	3:A:1675:HOH:O	2.12	0.48
1:B:276:LEU:CD2	1:B:276:LEU:N	2.74	0.48
1:C:523:LYS:HG2	3:C:876:HOH:O	2.12	0.48
1:D:377:ASN:HB2	1:D:381:TYR:O	2.12	0.48
1:D:528:MET:HE3	1:D:530:LEU:CD2	2.34	0.48
1:D:741:GLY:O	1:D:742:ILE:C	2.51	0.48
1:A:39:SER:O	1:A:40:ARG:O	2.31	0.48
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.48	0.48
1:C:102:ILE:HD13	1:C:116:LEU:HD22	1.94	0.48
1:D:60:LEU:HD12	1:D:60:LEU:C	2.34	0.48
1:A:704:HIS:HE1	1:A:711:VAL:O	1.96	0.48
1:C:172:ILE:H	1:C:186:THR:CG2	2.23	0.48
1:C:276:LEU:O	1:C:276:LEU:HD23	2.12	0.48
1:D:93:SER:HA	1:D:96:ASP:OD1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ALA:HA	3:A:849:HOH:O	2.11	0.48
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.96	0.48
1:C:74:ASN:HB3	1:C:92:ASN:HB3	1.96	0.48
1:C:458:SER:OG	1:C:471:ARG:HB2	2.13	0.48
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.34	0.48
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.28	0.48
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.49	0.48
1:A:140:ARG:HH11	1:A:140:ARG:CG	2.19	0.48
1:B:137:LEU:O	1:B:140:ARG:NH1	2.46	0.48
1:C:40:ARG:HH11	1:C:40:ARG:CG	2.26	0.48
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.97	0.48
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.49	0.48
1:D:413:ASP:HB3	1:D:414:TYR:CD1	2.48	0.48
1:D:415:LEU:HD13	1:D:415:LEU:C	2.34	0.48
1:A:291:ALA:O	1:A:295:ILE:HG23	2.13	0.48
1:D:160:VAL:HG23	1:D:161:GLY:H	1.77	0.48
1:B:39:SER:O	1:B:40:ARG:O	2.31	0.48
1:B:704:HIS:HE1	1:B:711:VAL:O	1.95	0.48
1:C:140:ARG:HG2	1:C:140:ARG:NH1	2.27	0.48
1:B:61:ARG:NH1	3:B:1551:HOH:O	2.45	0.48
1:B:187:TRP:N	1:B:187:TRP:CD1	2.81	0.48
1:B:276:LEU:H	1:B:276:LEU:HD22	1.79	0.48
1:B:379:GLU:HG3	3:B:1626:HOH:O	2.12	0.48
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.29	0.48
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.49	0.48
1:D:505:GLN:HB3	3:D:1471:HOH:O	2.13	0.48
1:D:74:ASN:HB3	1:D:92:ASN:CB	2.43	0.48
1:A:137:LEU:O	1:A:140:ARG:NH1	2.46	0.47
1:C:173:TYR:HB3	1:C:182:SER:OG	2.14	0.47
1:C:520:ASN:HA	3:C:1515:HOH:O	2.13	0.47
1:C:615:LYS:NZ	3:C:1144:HOH:O	2.38	0.47
1:D:74:ASN:HB3	1:D:92:ASN:HB3	1.95	0.47
1:D:459:VAL:HG22	1:D:460:SER:N	2.29	0.47
1:A:71:LYS:HE3	3:A:1782:HOH:O	2.14	0.47
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.44	0.47
1:B:253:ARG:HG3	3:B:1727:HOH:O	2.14	0.47
1:D:272:ASN:HD22	1:D:273:THR:N	2.12	0.47
1:A:97:GLU:HG2	3:A:1217:HOH:O	2.14	0.47
1:C:60:LEU:C	1:C:60:LEU:HD12	2.34	0.47
1:C:74:ASN:HB3	1:C:92:ASN:CB	2.43	0.47
1:D:51:ASN:HA	3:D:1204:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TRP:N	1:A:187:TRP:CD1	2.81	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.49	0.47
1:B:358:ARG:NH2	3:B:1305:HOH:O	2.46	0.47
1:C:272:ASN:HD22	1:C:273:THR:N	2.11	0.47
1:C:272:ASN:HD21	1:C:274:ASP:HB2	1.79	0.47
1:C:343:ARG:HD2	3:C:1044:HOH:O	2.13	0.47
1:C:691:ARG:NE	3:C:1662:HOH:O	2.30	0.47
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.79	0.47
1:A:281:ASN:HB3	3:A:1866:HOH:O	2.15	0.47
1:B:764:SER:HA	3:B:1050:HOH:O	2.14	0.47
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.39	0.47
1:C:741:GLY:O	1:C:742:ILE:C	2.52	0.47
1:D:102:ILE:HD13	1:D:116:LEU:HD22	1.95	0.47
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.50	0.47
1:D:726:VAL:O	1:D:726:VAL:HG13	2.15	0.47
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.35	0.47
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.44	0.47
1:A:85:ASN:ND2	3:A:1859:HOH:O	2.47	0.47
1:A:580:GLY:O	1:A:583:SER:HB2	2.15	0.47
1:B:71:LYS:HZ1	1:B:105:TYR:HB2	1.79	0.47
1:B:277:SER:O	1:B:278:SER:CB	2.61	0.47
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.50	0.47
1:C:40:ARG:HB2	1:C:506:ASN:O	2.15	0.47
1:C:276:LEU:CD2	1:C:276:LEU:N	2.75	0.47
1:A:392:LYS:HD2	1:A:393:ASP:N	2.29	0.47
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.96	0.47
1:C:40:ARG:NH1	1:C:505:GLN:O	2.47	0.47
1:C:429:ARG:NE	3:C:865:HOH:O	2.39	0.47
1:D:40:ARG:HB2	1:D:506:ASN:O	2.14	0.47
1:D:422:TYR:CD2	1:D:423:LYS:HD3	2.50	0.47
1:A:358:ARG:NH1	3:A:1346:HOH:O	2.46	0.47
1:D:272:ASN:HD21	1:D:274:ASP:HB2	1.80	0.47
1:A:407:ILE:CG2	1:A:415:LEU:HD21	2.45	0.47
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.35	0.47
1:A:276:LEU:H	1:A:276:LEU:HD22	1.78	0.47
1:C:93:SER:HA	1:C:96:ASP:OD1	2.14	0.47
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.35	0.47
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.79	0.47
1:D:483:HIS:HD2	3:D:1104:HOH:O	1.98	0.47
1:D:502:LYS:HD3	3:D:1101:HOH:O	2.15	0.47
1:A:140:ARG:NH1	1:A:140:ARG:CG	2.76	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:HB2	3:A:788:HOH:O	2.15	0.46
1:B:472:CYS:O	1:B:478:PRO:HA	2.15	0.46
1:D:458:SER:OG	1:D:471:ARG:HB2	2.15	0.46
1:A:366:LEU:HB3	3:A:1020:HOH:O	2.15	0.46
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.31	0.46
1:B:140:ARG:HH11	1:B:140:ARG:CG	2.19	0.46
1:B:310:ARG:NH1	1:B:329:ASP:OD1	2.49	0.46
1:B:726:VAL:O	1:B:726:VAL:CG1	2.63	0.46
1:C:459:VAL:HG22	1:C:460:SER:N	2.30	0.46
1:C:489:LYS:HG3	3:C:821:HOH:O	2.15	0.46
1:D:341:VAL:C	1:D:343:ARG:H	2.19	0.46
1:D:691:ARG:NE	3:D:1753:HOH:O	2.26	0.46
1:A:310:ARG:CZ	3:A:1515:HOH:O	2.61	0.46
1:C:354:VAL:HG12	3:C:1500:HOH:O	2.14	0.46
1:A:341:VAL:C	1:A:343:ARG:H	2.19	0.46
1:A:342:ALA:CB	3:A:1804:HOH:O	2.62	0.46
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.51	0.46
1:B:523:LYS:HD3	3:B:1814:HOH:O	2.15	0.46
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.51	0.46
1:C:271:VAL:HG23	1:C:283:THR:O	2.16	0.46
1:C:528:MET:HE3	1:C:530:LEU:CD2	2.35	0.46
1:D:69:LEU:HD11	1:D:107:ILE:HD12	1.96	0.46
1:B:159:PRO:HG3	3:B:1103:HOH:O	2.16	0.46
1:C:147:ARG:HD3	3:C:1473:HOH:O	2.15	0.46
1:C:415:LEU:C	1:C:415:LEU:HD13	2.36	0.46
1:C:538:LYS:HA	3:C:1265:HOH:O	2.15	0.46
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.36	0.46
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.50	0.46
1:D:358:ARG:NH2	3:D:951:HOH:O	2.48	0.46
1:D:382:ARG:NH2	3:D:802:HOH:O	2.47	0.46
1:A:74:ASN:HB2	3:A:1680:HOH:O	2.14	0.46
1:A:435:GLN:HE22	1:A:441:LYS:CD	2.27	0.46
1:B:41:LYS:HB2	3:B:1110:HOH:O	2.16	0.46
1:C:341:VAL:C	1:C:343:ARG:H	2.19	0.46
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.46
1:A:616:MET:HE1	3:A:1894:HOH:O	2.16	0.46
1:B:407:ILE:CG2	1:B:415:LEU:HD21	2.46	0.46
1:D:271:VAL:HG23	1:D:283:THR:O	2.15	0.46
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.98	0.46
1:A:276:LEU:H	1:A:276:LEU:HD23	1.80	0.46
1:C:69:LEU:HD11	1:C:107:ILE:HD12	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:ASN:ND2	3:C:1021:HOH:O	2.49	0.46
1:C:250:LYS:HE2	3:C:1224:HOH:O	2.15	0.46
1:C:388:GLN:CB	1:C:391:LYS:HB2	2.46	0.46
1:D:160:VAL:HG21	3:D:1571:HOH:O	2.15	0.46
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.51	0.46
1:D:764:SER:HB2	3:D:1325:HOH:O	2.16	0.46
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.52	0.45
1:A:186:THR:HG21	1:A:196:ASN:CB	2.46	0.45
1:A:454:CYS:HB2	3:A:1607:HOH:O	2.16	0.45
1:B:140:ARG:NH1	1:B:140:ARG:CG	2.76	0.45
1:B:562:ASN:HB2	3:B:826:HOH:O	2.17	0.45
1:D:334:SER:HB3	1:D:336:ARG:CD	2.46	0.45
1:A:546:VAL:HG22	1:A:547:TYR:N	2.31	0.45
1:A:721:LYS:HD3	1:B:736:THR:HG23	1.98	0.45
1:B:662:TYR:CE2	2:B:800:AAF:H132	2.51	0.45
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:C:310:ARG:HG3	1:C:329:ASP:OD1	2.16	0.45
1:D:40:ARG:NH1	1:D:505:GLN:O	2.50	0.45
1:D:276:LEU:CD2	1:D:276:LEU:N	2.74	0.45
1:B:341:VAL:C	1:B:343:ARG:H	2.19	0.45
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.50	0.45
1:C:186:THR:HG21	1:C:196:ASN:CB	2.47	0.45
1:D:186:THR:HG21	1:D:196:ASN:CB	2.47	0.45
1:D:498:SER:O	1:D:502:LYS:HG2	2.17	0.45
1:A:71:LYS:HE2	1:A:76:ILE:CD1	2.47	0.45
1:A:161:GLY:HA3	3:A:1154:HOH:O	2.17	0.45
1:B:71:LYS:HE2	1:B:76:ILE:CD1	2.46	0.45
1:B:546:VAL:HG22	1:B:547:TYR:N	2.30	0.45
1:D:310:ARG:HG3	1:D:329:ASP:OD1	2.16	0.45
1:D:413:ASP:HB3	1:D:414:TYR:HD1	1.82	0.45
1:A:61:ARG:HG3	3:A:1672:HOH:O	2.17	0.45
1:A:114:ILE:HD11	1:A:137:LEU:HD11	1.98	0.45
1:B:80:ASN:HB2	3:B:1465:HOH:O	2.17	0.45
1:B:325:MET:HE2	1:B:327:ILE:HG12	1.97	0.45
1:B:761:GLN:HE21	1:B:761:GLN:HB3	1.66	0.45
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.51	0.45
1:D:147:ARG:HD3	3:D:1078:HOH:O	2.15	0.45
1:D:489:LYS:HB3	1:D:489:LYS:HZ3	1.79	0.45
1:A:415:LEU:C	1:A:415:LEU:HD13	2.36	0.45
1:C:455:GLN:HA	3:C:1575:HOH:O	2.16	0.45
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ARG:HH22	1:D:253:ARG:HH22	1.64	0.45
1:C:334:SER:HB3	1:C:336:ARG:CD	2.46	0.45
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.99	0.45
1:C:658:ARG:HD2	1:C:661:TYR:CE1	2.51	0.45
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.52	0.45
1:C:512:LYS:HD3	3:C:948:HOH:O	2.16	0.45
1:B:110:ASP:HB3	1:B:112:GLN:HB2	1.99	0.45
1:D:388:GLN:CB	1:D:391:LYS:HB2	2.47	0.45
1:A:310:ARG:NH1	1:A:329:ASP:OD1	2.50	0.45
1:B:310:ARG:CZ	3:B:1167:HOH:O	2.65	0.45
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.47	0.45
1:B:579:ASP:HB3	1:B:583:SER:OG	2.17	0.45
1:D:306:ALA:HB3	1:D:310:ARG:HD2	1.98	0.45
1:B:50:LYS:HE3	3:B:1636:HOH:O	2.16	0.44
1:B:186:THR:HG21	1:B:196:ASN:CB	2.47	0.44
1:D:147:ARG:NH1	3:D:1473:HOH:O	2.50	0.44
1:B:107:ILE:HG12	1:B:114:ILE:HG12	1.99	0.44
1:B:276:LEU:H	1:B:276:LEU:HD23	1.80	0.44
1:B:697:GLN:NE2	3:B:1646:HOH:O	2.39	0.44
1:C:141:GLN:HA	3:C:1319:HOH:O	2.16	0.44
1:C:513:LYS:O	1:C:527:GLN:HA	2.17	0.44
1:A:442:VAL:HG11	3:A:1768:HOH:O	2.17	0.44
1:A:504:LEU:HA	1:A:507:VAL:CG1	2.48	0.44
1:D:513:LYS:O	1:D:527:GLN:HA	2.17	0.44
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.44
1:A:231:THR:HG22	1:A:232:GLU:HG3	2.00	0.44
1:A:651:ILE:HG21	1:A:755:MET:HE2	1.99	0.44
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.46	0.44
1:A:726:VAL:O	1:A:726:VAL:CG1	2.64	0.44
1:B:136:ASP:OD1	1:B:138:ASN:HB2	2.17	0.44
1:B:580:GLY:O	1:B:583:SER:HB2	2.17	0.44
1:D:492:ARG:HA	3:D:1752:HOH:O	2.17	0.44
1:A:489:LYS:HB3	1:A:489:LYS:HZ2	1.81	0.44
1:B:114:ILE:HD11	1:B:137:LEU:HD11	1.99	0.44
1:B:377:ASN:ND2	3:B:827:HOH:O	2.49	0.44
1:B:717:ALA:HA	3:B:1870:HOH:O	2.17	0.44
1:C:498:SER:O	1:C:502:LYS:HG2	2.17	0.44
1:B:415:LEU:HD13	1:B:415:LEU:C	2.38	0.44
1:C:108:SER:C	1:C:110:ASP:N	2.71	0.44
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.99	0.44
1:C:704:HIS:HE1	1:C:711:VAL:O	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:VAL:HG13	1:C:726:VAL:O	2.17	0.44
1:D:471:ARG:HG2	1:D:480:TYR:CD2	2.53	0.44
1:A:152:THR:HG21	1:A:155:VAL:CG2	2.48	0.44
1:A:471:ARG:HG3	3:A:1510:HOH:O	2.18	0.44
1:B:152:THR:HG21	1:B:155:VAL:CG2	2.47	0.44
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.53	0.44
1:C:734:TRP:CD1	1:C:736:THR:HG22	2.53	0.44
1:D:319:ILE:HD11	1:D:673:LEU:CD1	2.48	0.44
1:D:388:GLN:HG2	1:D:391:LYS:HD3	2.00	0.44
1:D:658:ARG:HD2	1:D:661:TYR:CE1	2.52	0.44
1:B:106:SER:HB3	1:B:115:LEU:HB3	2.00	0.43
1:C:306:ALA:HB3	1:C:310:ARG:HD2	1.99	0.43
1:C:321:ASN:ND2	3:C:1389:HOH:O	2.50	0.43
1:C:697:GLN:HG3	3:C:1475:HOH:O	2.18	0.43
1:D:78:VAL:HG13	1:D:78:VAL:O	2.18	0.43
1:D:172:ILE:H	1:D:186:THR:CG2	2.24	0.43
1:D:243:ASP:HB3	3:D:1071:HOH:O	2.17	0.43
1:D:343:ARG:NH2	3:D:905:HOH:O	2.49	0.43
1:D:505:GLN:HB3	3:D:822:HOH:O	2.19	0.43
1:A:107:ILE:HG12	1:A:114:ILE:HG12	2.00	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.82	0.43
1:B:336:ARG:H	1:B:336:ARG:HG3	1.65	0.43
1:B:489:LYS:HB3	1:B:489:LYS:HZ2	1.83	0.43
1:C:184:ARG:HD2	1:C:187:TRP:CD2	2.52	0.43
1:C:516:PHE:CE2	1:C:523:LYS:HE2	2.53	0.43
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.46	0.43
1:D:52:THR:HG22	3:D:1187:HOH:O	2.18	0.43
1:D:697:GLN:HG3	3:D:1488:HOH:O	2.17	0.43
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.53	0.43
1:C:388:GLN:HG2	1:C:391:LYS:HD3	2.00	0.43
1:D:546:VAL:HG22	1:D:547:TYR:N	2.33	0.43
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.53	0.43
1:B:435:GLN:NE2	1:B:441:LYS:HD3	2.34	0.43
1:B:609:ALA:HA	3:B:1143:HOH:O	2.17	0.43
1:D:310:ARG:NH1	1:D:329:ASP:OD1	2.52	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.99	0.43
1:B:487:ASN:O	1:B:488:ASP:HB2	2.17	0.43
1:C:89:PHE:CD1	1:C:90:LEU:HD12	2.35	0.43
1:C:413:ASP:HB3	1:C:414:TYR:HD1	1.82	0.43
1:C:721:LYS:NZ	3:C:1313:HOH:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:PHE:CD2	1:D:100:HIS:HB2	2.53	0.43
1:D:147:ARG:HD2	3:D:1523:HOH:O	2.18	0.43
1:A:110:ASP:HB3	1:A:112:GLN:HB2	1.99	0.43
1:C:98:PHE:CD2	1:C:100:HIS:HB2	2.53	0.43
1:C:319:ILE:HD11	1:C:673:LEU:CD1	2.48	0.43
1:D:520:ASN:O	1:D:521:GLU:HB2	2.19	0.43
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.54	0.43
1:B:183:TYR:HE1	1:B:277:SER:C	2.22	0.43
1:B:377:ASN:HB3	1:B:379:GLU:H	1.83	0.43
1:C:147:ARG:HB2	3:C:1018:HOH:O	2.19	0.43
1:C:310:ARG:NH1	1:C:329:ASP:OD1	2.52	0.43
1:C:546:VAL:HG22	1:C:547:TYR:N	2.34	0.43
1:C:718:GLN:HA	1:C:718:GLN:HE21	1.84	0.43
1:A:253:ARG:HG3	3:A:1821:HOH:O	2.18	0.43
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.41	0.43
1:B:435:GLN:HE22	1:B:441:LYS:CD	2.32	0.43
1:D:92:ASN:HA	3:D:1633:HOH:O	2.19	0.43
1:A:187:TRP:CZ2	3:A:1866:HOH:O	2.72	0.42
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.42
1:B:388:GLN:HB2	3:B:1831:HOH:O	2.18	0.42
1:B:536:LYS:NZ	1:B:536:LYS:HB3	2.34	0.42
1:C:183:TYR:CE2	1:C:276:LEU:HG	2.54	0.42
1:C:237:GLU:HA	1:C:252:VAL:O	2.20	0.42
1:C:289:ALA:CB	1:C:290:PRO:HA	2.25	0.42
1:C:379:GLU:HG2	3:C:1061:HOH:O	2.19	0.42
1:C:422:TYR:CZ	1:C:423:LYS:HE3	2.54	0.42
1:C:503:MET:HE3	3:C:1625:HOH:O	2.18	0.42
1:D:492:ARG:HD3	3:D:889:HOH:O	2.19	0.42
1:A:106:SER:HB3	1:A:115:LEU:HB3	2.00	0.42
1:A:487:ASN:O	1:A:488:ASP:HB2	2.19	0.42
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.53	0.42
1:C:78:VAL:HG13	1:C:78:VAL:O	2.20	0.42
1:C:111:GLY:O	1:C:137:LEU:HD12	2.19	0.42
1:C:319:ILE:C	1:C:321:ASN:H	2.22	0.42
1:C:520:ASN:O	1:C:521:GLU:HB2	2.19	0.42
1:D:415:LEU:HB3	1:D:434:ILE:CG2	2.49	0.42
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.20	0.42
1:A:458:SER:OG	1:A:471:ARG:HB2	2.19	0.42
1:B:630:SER:HA	1:B:654:ALA:O	2.20	0.42
1:D:184:ARG:HD2	1:D:187:TRP:CD2	2.53	0.42
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:ILE:HA	3:D:1680:HOH:O	2.19	0.42
1:A:536:LYS:NZ	1:A:536:LYS:HB3	2.33	0.42
1:B:331:ASP:HB3	1:B:334:SER:HB2	2.01	0.42
1:C:334:SER:CB	1:C:336:ARG:HD2	2.49	0.42
1:C:513:LYS:HE3	3:C:1577:HOH:O	2.18	0.42
1:C:660:GLU:HG3	3:C:800:HOH:O	2.20	0.42
1:D:336:ARG:H	1:D:336:ARG:HD2	1.85	0.42
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.19	0.42
1:B:175:LYS:NZ	3:B:1555:HOH:O	2.51	0.42
1:B:528:MET:HB2	1:B:528:MET:HE2	1.93	0.42
1:B:533:HIS:HD2	3:B:1851:HOH:O	2.00	0.42
1:B:691:ARG:NH2	3:B:1749:HOH:O	2.53	0.42
1:C:54:ARG:HE	1:C:54:ARG:HB2	1.69	0.42
1:D:40:ARG:HE	1:D:508:GLN:HG2	1.85	0.42
1:D:111:GLY:O	1:D:137:LEU:HD12	2.19	0.42
1:D:734:TRP:CD1	1:D:736:THR:HG22	2.54	0.42
1:A:334:SER:HB3	1:A:336:ARG:CD	2.50	0.42
1:B:334:SER:HB3	1:B:336:ARG:CD	2.50	0.42
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.95	0.42
1:B:532:PRO:HD3	1:B:569:SER:HA	2.02	0.42
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.54	0.42
1:C:536:LYS:NZ	1:C:536:LYS:CB	2.83	0.42
1:D:358:ARG:NE	3:D:1587:HOH:O	2.52	0.42
1:B:247:GLN:NE2	3:B:1915:HOH:O	2.52	0.42
1:B:658:ARG:HB3	1:B:689:MET:HE1	2.02	0.42
1:C:336:ARG:HD2	1:C:336:ARG:H	1.85	0.42
1:D:334:SER:CB	1:D:336:ARG:HD2	2.49	0.42
1:D:375:ILE:HB	3:D:1766:HOH:O	2.18	0.42
1:D:486:VAL:CG1	1:D:487:ASN:N	2.82	0.42
1:D:718:GLN:HA	1:D:718:GLN:NE2	2.35	0.42
1:A:579:ASP:HB3	1:A:583:SER:OG	2.20	0.42
1:B:231:THR:HG22	1:B:232:GLU:HG3	2.02	0.42
1:C:342:ALA:HA	3:C:1288:HOH:O	2.20	0.42
1:C:415:LEU:HB3	1:C:434:ILE:CG2	2.50	0.42
1:D:57:LEU:HB3	3:D:1319:HOH:O	2.19	0.42
1:D:183:TYR:CE2	1:D:276:LEU:HG	2.54	0.42
1:D:505:GLN:HB2	3:D:1750:HOH:O	2.19	0.42
1:A:183:TYR:HE1	1:A:277:SER:C	2.23	0.41
1:A:282:ALA:HB1	3:A:1288:HOH:O	2.19	0.41
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.92	0.41
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ALA:HB3	3:C:1103:HOH:O	2.18	0.41
1:C:679:ASN:ND2	3:C:1017:HOH:O	2.53	0.41
1:D:65:ASP:CG	1:D:464:GLU:HB2	2.40	0.41
1:D:108:SER:C	1:D:110:ASP:N	2.71	0.41
1:A:177:GLU:CB	1:A:180:LEU:HD22	2.43	0.41
1:A:512:LYS:HD3	3:A:1077:HOH:O	2.20	0.41
1:B:704:HIS:CE1	1:B:711:VAL:O	2.73	0.41
1:C:40:ARG:HE	1:C:508:GLN:HG2	1.85	0.41
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.40	0.41
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.55	0.41
1:D:54:ARG:HE	1:D:54:ARG:HB2	1.69	0.41
1:D:89:PHE:CD1	1:D:90:LEU:HD12	2.35	0.41
1:D:422:TYR:CZ	1:D:423:LYS:HE3	2.55	0.41
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.56	0.41
1:A:532:PRO:HD3	1:A:569:SER:HA	2.02	0.41
1:B:366:LEU:HD12	3:B:1691:HOH:O	2.21	0.41
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.02	0.41
1:C:615:LYS:HG2	3:C:1144:HOH:O	2.21	0.41
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.36	0.41
1:C:388:GLN:HB2	1:C:391:LYS:HB2	2.02	0.41
1:D:283:THR:HG22	1:D:285:ILE:HD12	2.03	0.41
1:D:289:ALA:CB	1:D:290:PRO:CA	2.89	0.41
1:C:91:GLU:HB2	3:C:1085:HOH:O	2.21	0.41
1:A:175:LYS:HE3	1:A:180:LEU:O	2.21	0.41
1:B:60:LEU:C	1:B:60:LEU:HD12	2.41	0.41
1:B:160:VAL:CG2	1:B:161:GLY:N	2.83	0.41
1:C:542:LEU:C	1:C:542:LEU:HD23	2.41	0.41
1:C:392:LYS:HB3	3:C:1446:HOH:O	2.19	0.41
1:C:658:ARG:HD2	1:C:661:TYR:CZ	2.56	0.41
1:D:319:ILE:C	1:D:321:ASN:H	2.21	0.41
1:D:388:GLN:HB2	1:D:391:LYS:HB2	2.03	0.41
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.55	0.41
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.56	0.41
1:C:358:ARG:NH2	3:C:943:HOH:O	2.52	0.41
1:C:487:ASN:HB2	3:C:821:HOH:O	2.20	0.41
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.55	0.41
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.02	0.41
1:D:536:LYS:NZ	1:D:536:LYS:CB	2.84	0.41
1:A:40:ARG:NH1	3:A:1508:HOH:O	2.54	0.41
1:A:82:GLU:HG2	1:A:83:TYR:CZ	2.55	0.41
1:A:276:LEU:HD23	1:A:276:LEU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:SER:O	1:C:350:THR:HB	2.20	0.41
1:A:691:ARG:NE	3:A:1911:HOH:O	2.21	0.41
1:B:71:LYS:HE2	1:B:76:ILE:HD13	2.03	0.41
1:B:76:ILE:HB	1:B:90:LEU:HD12	2.03	0.41
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.56	0.41
1:C:147:ARG:HH11	1:C:147:ARG:HG2	1.86	0.41
1:C:237:GLU:OE2	1:C:253:ARG:NH2	2.47	0.41
1:C:630:SER:OG	3:C:1661:HOH:O	2.20	0.41
1:D:285:ILE:HD12	1:D:285:ILE:N	2.36	0.41
1:D:429:ARG:NE	3:D:876:HOH:O	2.48	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.02	0.41
1:A:60:LEU:HD12	1:A:60:LEU:C	2.41	0.41
1:A:331:ASP:HB3	1:A:334:SER:HB2	2.02	0.41
1:A:685:ASN:ND2	3:A:1196:HOH:O	2.51	0.41
1:B:78:VAL:HG13	1:B:78:VAL:O	2.20	0.41
1:B:175:LYS:HE3	1:B:180:LEU:O	2.21	0.41
1:B:325:MET:HE1	1:B:327:ILE:HD11	2.02	0.41
1:C:384:ILE:HG13	1:C:404:VAL:HG21	2.02	0.41
1:A:409:ALA:O	1:A:415:LEU:HD22	2.21	0.40
1:A:704:HIS:CE1	1:A:711:VAL:O	2.73	0.40
1:B:369:ASN:ND2	3:B:1167:HOH:O	2.53	0.40
1:C:283:THR:HG22	1:C:285:ILE:HD12	2.02	0.40
1:D:489:LYS:HG3	3:D:1169:HOH:O	2.20	0.40
1:D:726:VAL:CG1	1:D:726:VAL:O	2.69	0.40
1:A:413:ASP:HB3	1:A:414:TYR:CD1	2.56	0.40
1:B:155:VAL:HG22	1:B:166:TYR:HB2	2.03	0.40
1:D:160:VAL:O	1:D:161:GLY:O	2.39	0.40
1:A:90:LEU:HD22	1:A:91:GLU:O	2.22	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.96	0.40
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.04	0.40
1:B:411:THR:HG21	3:B:1314:HOH:O	2.20	0.40
1:D:85:ASN:ND2	3:D:1371:HOH:O	2.50	0.40
1:D:507:VAL:HB	3:D:1760:HOH:O	2.21	0.40
1:A:217:SER:HB3	1:A:222:PHE:HB2	2.03	0.40
1:A:543:LEU:HD12	1:A:567:LEU:HD13	2.03	0.40
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.56	0.40
1:D:658:ARG:HD2	1:D:661:TYR:CZ	2.56	0.40
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.70	0.40
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.52	0.40
1:A:513:LYS:O	1:A:527:GLN:HA	2.22	0.40
1:A:693:GLU:HB2	3:A:965:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ALA:O	1:C:492:ARG:NH2	2.54	0.40
1:C:108:SER:C	1:C:110:ASP:H	2.25	0.40
1:C:630:SER:HA	1:C:654:ALA:O	2.21	0.40
1:C:696:LYS:NZ	3:C:1402:HOH:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	724/726 (100%)	678 (94%)	39 (5%)	7 (1%)	13	8
1	B	724/726 (100%)	678 (94%)	39 (5%)	7 (1%)	13	8
1	C	724/726 (100%)	677 (94%)	40 (6%)	7 (1%)	13	8
1	D	724/726 (100%)	676 (93%)	41 (6%)	7 (1%)	13	8
All	All	2896/2904 (100%)	2709 (94%)	159 (6%)	28 (1%)	13	8

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	278	SER
1	B	40	ARG
1	B	278	SER
1	C	40	ARG
1	C	278	SER
1	D	40	ARG
1	D	278	SER
1	A	161	GLY
1	A	289	ALA
1	B	161	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	289	ALA
1	C	161	GLY
1	C	289	ALA
1	C	320	GLN
1	D	161	GLY
1	D	289	ALA
1	D	320	GLN
1	A	520	ASN
1	B	520	ASN
1	A	320	GLN
1	B	320	GLN
1	C	520	ASN
1	D	520	ASN
1	C	334	SER
1	D	334	SER
1	A	94	THR
1	B	94	THR

5.3.2 Protein sidechains ⓘ

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	651/651 (100%)	603 (93%)	48 (7%)	11	8
1	B	651/651 (100%)	605 (93%)	46 (7%)	12	9
1	C	651/651 (100%)	609 (94%)	42 (6%)	14	11
1	D	651/651 (100%)	610 (94%)	41 (6%)	15	12
All	All	2604/2604 (100%)	2427 (93%)	177 (7%)	13	10

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	41	LYS
1	A	51	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	57	LEU
1	A	66	HIS
1	A	73	GLU
1	A	90	LEU
1	A	91	GLU
1	A	92	ASN
1	A	110	ASP
1	A	140	ARG
1	A	141	GLN
1	A	170	ASN
1	A	207	VAL
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	272	ASN
1	A	276	LEU
1	A	285	ILE
1	A	303	VAL
1	A	313	LEU
1	A	336	ARG
1	A	358	ARG
1	A	361	GLU
1	A	385	CYS
1	A	388	GLN
1	A	392	LYS
1	A	413	ASP
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	482	LEU
1	A	514	LEU
1	A	520	ASN
1	A	523	LYS
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	583	SER
1	A	603	VAL
1	A	658	ARG
1	A	673	LEU
1	A	679	ASN
1	A	701	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	702	LEU
1	A	761	GLN
1	B	39	SER
1	B	40	ARG
1	B	41	LYS
1	B	51	ASN
1	B	57	LEU
1	B	66	HIS
1	B	73	GLU
1	B	90	LEU
1	B	91	GLU
1	B	92	ASN
1	B	110	ASP
1	B	140	ARG
1	B	141	GLN
1	B	170	ASN
1	B	207	VAL
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	272	ASN
1	B	276	LEU
1	B	285	ILE
1	B	313	LEU
1	B	336	ARG
1	B	361	GLU
1	B	385	CYS
1	B	388	GLN
1	B	392	LYS
1	B	413	ASP
1	B	436	LEU
1	B	440	THR
1	B	448	GLU
1	B	482	LEU
1	B	514	LEU
1	B	520	ASN
1	B	523	LYS
1	B	536	LYS
1	B	543	LEU
1	B	561	LEU
1	B	583	SER
1	B	603	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	658	ARG
1	B	673	LEU
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	761	GLN
1	C	40	ARG
1	C	41	LYS
1	C	51	ASN
1	C	73	GLU
1	C	90	LEU
1	C	110	ASP
1	C	145	GLU
1	C	160	VAL
1	C	170	ASN
1	C	207	VAL
1	C	246	LEU
1	C	253	ARG
1	C	254	VAL
1	C	272	ASN
1	C	276	LEU
1	C	303	VAL
1	C	326	ASP
1	C	332	GLU
1	C	336	ARG
1	C	385	CYS
1	C	388	GLN
1	C	392	LYS
1	C	436	LEU
1	C	440	THR
1	C	448	GLU
1	C	482	LEU
1	C	505	GLN
1	C	514	LEU
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU
1	C	561	LEU
1	C	566	TYR
1	C	583	SER
1	C	603	VAL
1	C	658	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	679	ASN
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	736	THR
1	C	761	GLN
1	D	40	ARG
1	D	41	LYS
1	D	51	ASN
1	D	73	GLU
1	D	90	LEU
1	D	110	ASP
1	D	145	GLU
1	D	160	VAL
1	D	170	ASN
1	D	207	VAL
1	D	246	LEU
1	D	253	ARG
1	D	254	VAL
1	D	272	ASN
1	D	276	LEU
1	D	303	VAL
1	D	326	ASP
1	D	332	GLU
1	D	336	ARG
1	D	385	CYS
1	D	392	LYS
1	D	436	LEU
1	D	440	THR
1	D	448	GLU
1	D	482	LEU
1	D	505	GLN
1	D	514	LEU
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	561	LEU
1	D	566	TYR
1	D	583	SER
1	D	603	VAL
1	D	658	ARG
1	D	679	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	736	THR
1	D	761	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	75	ASN
1	A	92	ASN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	435	GLN
1	A	483	HIS
1	A	533	HIS
1	A	572	ASN
1	A	606	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	51	ASN
1	B	72	GLN
1	B	75	ASN
1	B	92	ASN
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	345	HIS
1	B	369	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	435	GLN
1	B	483	HIS
1	B	533	HIS
1	B	572	ASN
1	B	606	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	GLN
1	C	51	ASN
1	C	169	ASN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	314	GLN
1	C	369	ASN
1	C	377	ASN
1	C	388	GLN
1	C	483	HIS
1	C	487	ASN
1	C	533	HIS
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	761	GLN
1	D	51	ASN
1	D	123	GLN
1	D	169	ASN
1	D	170	ASN
1	D	272	ASN
1	D	314	GLN
1	D	369	ASN
1	D	377	ASN
1	D	388	GLN
1	D	483	HIS
1	D	487	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	533	HIS
1	D	572	ASN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	761	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
2	AAF	B	800	1	31,31,31	1.48	7 (22%)	37,42,42	1.08	4 (10%)

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	AAF	B	800	1	-	2/25/44/44	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	AAF	C1-N8	3.05	1.41	1.34
2	B	800	AAF	C14-C10	2.85	1.56	1.53
2	B	800	AAF	C25-C20	2.83	1.44	1.39
2	B	800	AAF	C14-N18	-2.78	1.34	1.48
2	B	800	AAF	C22-C23	2.58	1.43	1.39
2	B	800	AAF	C24-C23	2.43	1.43	1.39
2	B	800	AAF	C22-C21	2.28	1.42	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	AAF	C12-C13-N8	2.40	107.36	103.24
2	B	800	AAF	C29-O28-C26	2.39	120.40	115.81
2	B	800	AAF	C11-C10-C14	-2.29	103.61	112.17
2	B	800	AAF	C14-C10-N8	2.25	118.39	110.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	800	AAF	N8-C10-C14-N18
2	B	800	AAF	C11-C10-C14-N18

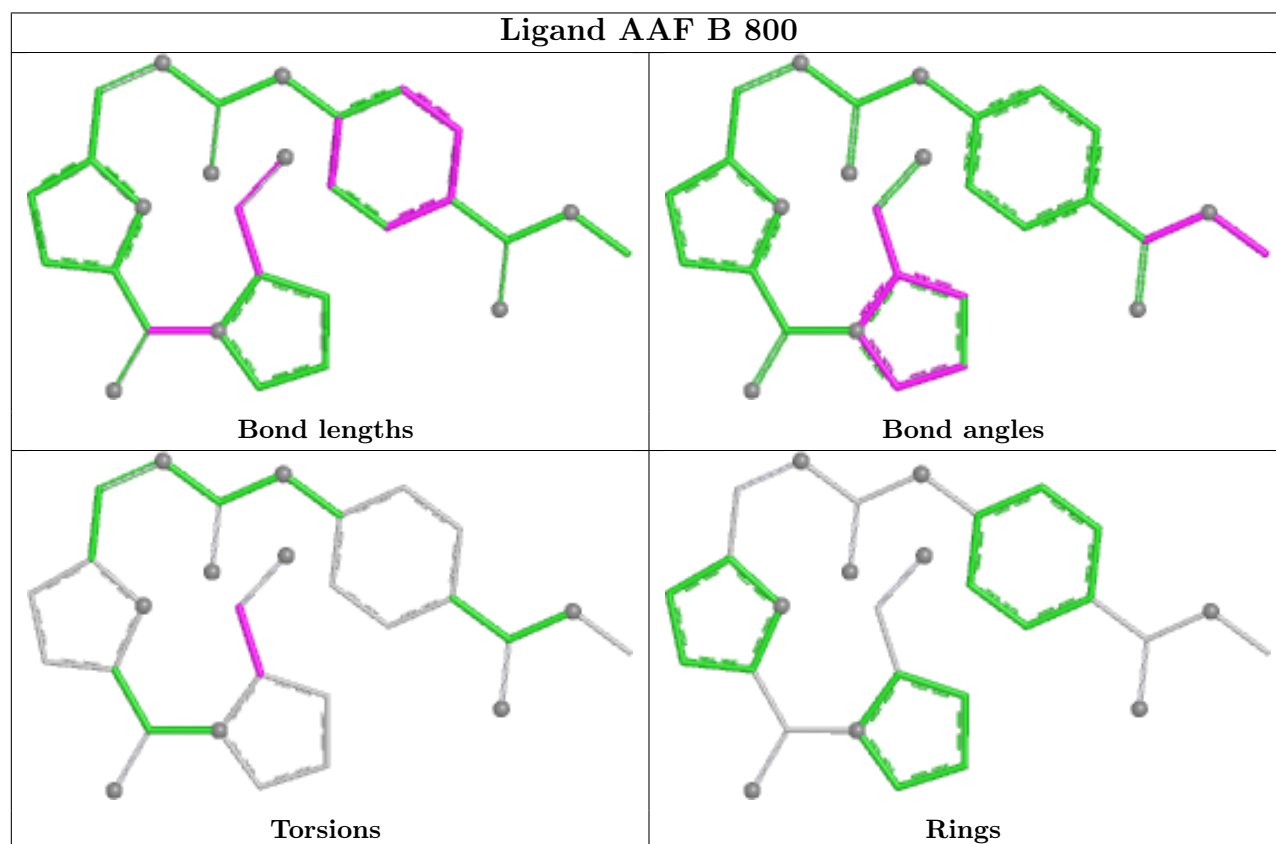
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	AAF	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/726 (100%)	0.44	68 (9%) 15 14	16, 27, 56, 88	0
1	B	726/726 (100%)	0.53	86 (11%) 10 9	15, 28, 63, 85	0
1	C	726/726 (100%)	0.33	41 (5%) 31 29	18, 34, 61, 79	0
1	D	726/726 (100%)	0.31	44 (6%) 28 26	18, 32, 60, 79	0
All	All	2904/2904 (100%)	0.40	239 (8%) 19 17	15, 30, 60, 88	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	12.0
1	A	282	ALA	8.1
1	A	280	THR	7.9
1	D	289	ALA	6.5
1	A	281	ASN	6.5
1	A	342	ALA	6.4
1	B	111	GLY	6.3
1	B	341	VAL	6.0
1	A	278	SER	5.7
1	B	277	SER	5.3
1	A	277	SER	5.0
1	A	289	ALA	4.9
1	D	342	ALA	4.7
1	B	39	SER	4.7
1	C	277	SER	4.6
1	B	160	VAL	4.5
1	A	333	SER	4.5
1	A	276	LEU	4.5
1	C	333	SER	4.5
1	B	342	ALA	4.2
1	B	71	LYS	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	39	SER	4.1
1	D	39	SER	4.1
1	C	71	LYS	4.0
1	D	621	ASN	4.0
1	C	105	TYR	4.0
1	A	412	SER	4.0
1	B	114	ILE	4.0
1	D	90	LEU	4.0
1	B	278	SER	3.9
1	B	289	ALA	3.9
1	C	289	ALA	3.8
1	A	114	ILE	3.8
1	B	103	ASN	3.7
1	C	138	ASN	3.6
1	B	66	HIS	3.6
1	A	283	THR	3.6
1	A	377	ASN	3.6
1	C	520	ASN	3.6
1	D	276	LEU	3.5
1	D	520	ASN	3.5
1	A	72	GLN	3.5
1	A	645	GLY	3.5
1	B	90	LEU	3.5
1	A	74	ASN	3.4
1	A	366	LEU	3.4
1	B	105	TYR	3.4
1	B	72	GLN	3.4
1	B	137	LEU	3.4
1	A	392	LYS	3.4
1	B	413	ASP	3.4
1	A	90	LEU	3.3
1	A	538	LYS	3.3
1	B	143	ILE	3.3
1	B	73	GLU	3.3
1	B	321	ASN	3.3
1	D	160	VAL	3.3
1	A	413	ASP	3.2
1	A	103	ASN	3.2
1	A	71	LYS	3.2
1	B	764	SER	3.2
1	D	71	LYS	3.2
1	B	109	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	139	LYS	3.2
1	C	390	ASP	3.2
1	C	88	VAL	3.1
1	C	98	PHE	3.1
1	D	277	SER	3.1
1	A	161	GLY	3.1
1	D	92	ASN	3.1
1	A	73	GLU	3.1
1	B	76	ILE	3.1
1	D	334	SER	3.1
1	D	279	VAL	3.1
1	B	366	LEU	3.1
1	B	330	TYR	3.1
1	C	389	ILE	3.0
1	B	61	ARG	3.0
1	A	341	VAL	3.0
1	B	97	GLU	3.0
1	A	39	SER	3.0
1	B	40	ARG	3.0
1	B	377	ASN	3.0
1	A	140	ARG	3.0
1	B	282	ALA	3.0
1	B	63	ILE	2.9
1	B	134	ILE	2.9
1	A	187	TRP	2.9
1	B	276	LEU	2.9
1	B	412	SER	2.9
1	B	333	SER	2.9
1	D	72	GLN	2.9
1	B	340	LEU	2.9
1	D	333	SER	2.9
1	A	487	ASN	2.9
1	D	40	ARG	2.9
1	D	61	ARG	2.9
1	C	276	LEU	2.8
1	B	440	THR	2.8
1	B	159	PRO	2.8
1	B	180	LEU	2.8
1	B	336	ARG	2.8
1	B	367	ASP	2.8
1	B	442	VAL	2.8
1	B	334	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	391	LYS	2.7
1	B	466	LYS	2.7
1	A	334	SER	2.7
1	B	487	ASN	2.7
1	B	307	THR	2.7
1	A	110	ASP	2.7
1	C	182	SER	2.7
1	D	74	ASN	2.7
1	C	72	GLN	2.7
1	C	536	LYS	2.7
1	A	92	ASN	2.7
1	B	343	ARG	2.7
1	B	411	THR	2.7
1	C	341	VAL	2.6
1	B	443	THR	2.6
1	D	280	THR	2.6
1	C	110	ASP	2.6
1	A	518	ILE	2.6
1	C	391	LYS	2.6
1	B	138	ASN	2.6
1	D	615	LYS	2.6
1	A	102	ILE	2.6
1	C	114	ILE	2.6
1	C	764	SER	2.6
1	A	160	VAL	2.6
1	B	120	TYR	2.6
1	B	414	TYR	2.5
1	A	440	THR	2.5
1	B	280	THR	2.5
1	A	520	ASN	2.5
1	B	107	ILE	2.5
1	D	412	SER	2.5
1	B	62	TRP	2.5
1	D	380	GLY	2.5
1	D	423	LYS	2.5
1	D	88	VAL	2.5
1	A	105	TYR	2.5
1	B	69	LEU	2.5
1	C	336	ARG	2.5
1	B	74	ASN	2.5
1	B	102	ILE	2.5
1	A	321	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	614	SER	2.4
1	A	764	SER	2.4
1	B	217	SER	2.4
1	C	40	ARG	2.4
1	B	337	TRP	2.4
1	B	281	ASN	2.4
1	B	505	GLN	2.4
1	D	77	LEU	2.4
1	D	697	GLN	2.4
1	A	41	LYS	2.4
1	A	489	LYS	2.4
1	C	160	VAL	2.4
1	C	275	SER	2.4
1	D	86	SER	2.4
1	C	102	ILE	2.4
1	B	462	SER	2.4
1	B	75	ASN	2.3
1	A	507	VAL	2.3
1	D	764	SER	2.3
1	B	132	TYR	2.3
1	C	321	ASN	2.3
1	C	377	ASN	2.3
1	D	442	VAL	2.3
1	D	89	PHE	2.3
1	A	340	LEU	2.3
1	B	116	LEU	2.3
1	C	340	LEU	2.3
1	A	335	GLY	2.3
1	A	138	ASN	2.3
1	A	218	PRO	2.2
1	B	178	PRO	2.2
1	D	91	GLU	2.2
1	C	74	ASN	2.2
1	B	101	SER	2.2
1	B	139	LYS	2.2
1	B	392	LYS	2.2
1	A	40	ARG	2.2
1	C	75	ASN	2.2
1	D	321	ASN	2.2
1	D	336	ARG	2.2
1	B	187	TRP	2.2
1	B	435	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	137	LEU	2.2
1	B	68	TYR	2.2
1	B	275	SER	2.2
1	B	615	LYS	2.2
1	B	486	VAL	2.2
1	B	145	GLU	2.2
1	B	327	ILE	2.2
1	C	73	GLU	2.2
1	A	505	GLN	2.2
1	B	482	LEU	2.1
1	A	523	LYS	2.1
1	C	334	SER	2.1
1	B	467	TYR	2.1
1	B	339	CYS	2.1
1	A	95	PHE	2.1
1	A	147	ARG	2.1
1	D	140	ARG	2.1
1	D	281	ASN	2.1
1	C	141	GLN	2.1
1	A	332	GLU	2.1
1	D	147	ARG	2.1
1	A	437	SER	2.1
1	B	370	SER	2.1
1	B	389	ILE	2.1
1	D	52	THR	2.1
1	A	66	HIS	2.1
1	C	92	ASN	2.1
1	C	187	TRP	2.1
1	D	83	TYR	2.1
1	C	507	VAL	2.1
1	A	441	LYS	2.1
1	B	110	ASP	2.1
1	C	614	SER	2.1
1	D	93	SER	2.1
1	D	436	LEU	2.1
1	B	465	ALA	2.0
1	C	506	ASN	2.0
1	B	56	LYS	2.0
1	A	275	SER	2.0
1	D	278	SER	2.0
1	A	141	GLN	2.0
1	C	482	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	508	GLN	2.0
1	A	521	GLU	2.0
1	A	506	ASN	2.0
1	A	336	ARG	2.0
1	C	538	LYS	2.0
1	D	386	TYR	2.0
1	A	442	VAL	2.0
1	A	104	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

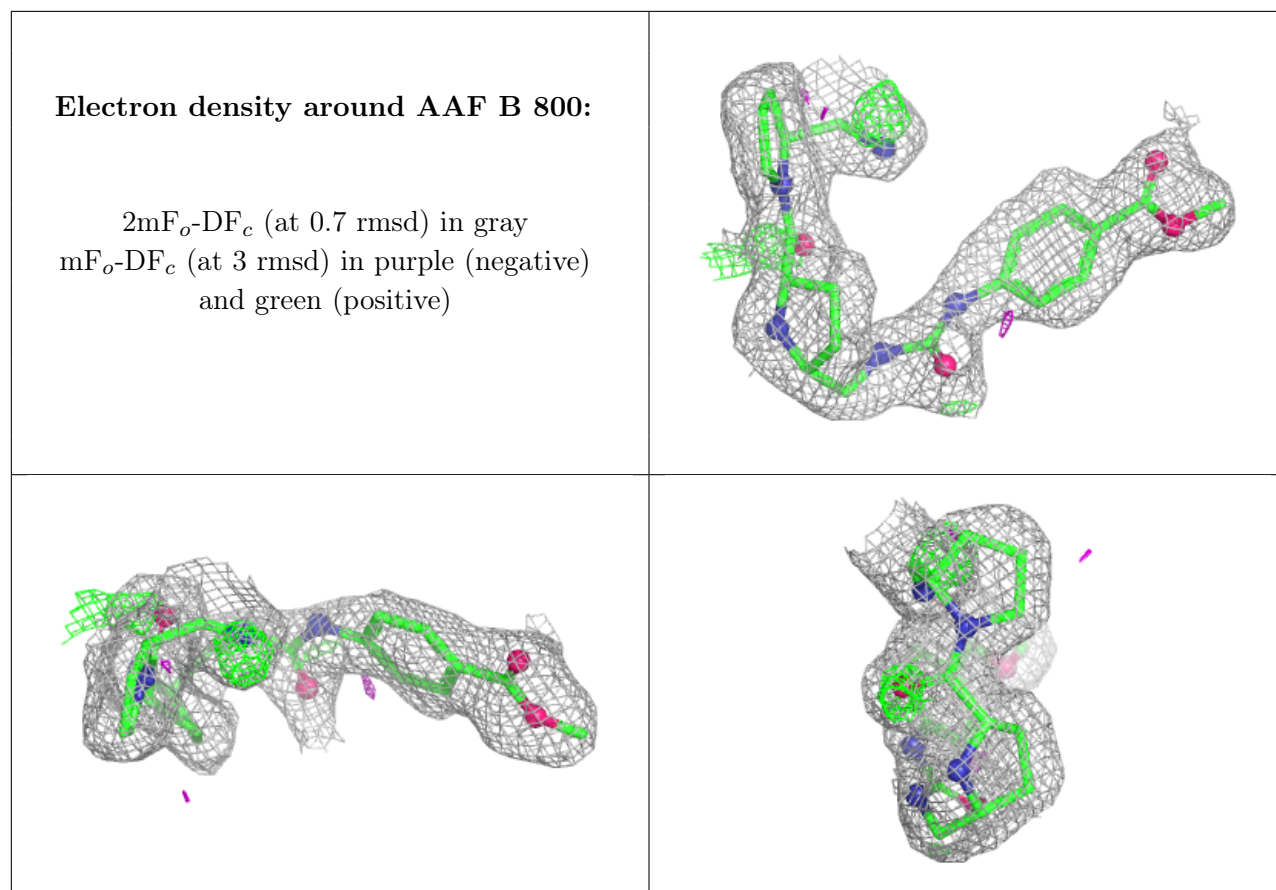
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	AAF	B	800	29/29	0.91	0.10	26,31,48,50	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 ⓘ

There are no such residues in this entry.