



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 11:54 PM EDT

PDB ID : 2G97
Title : Crystal Structure of Visfatin/Pre-B Cell Colony Enhancing Factor 1/Nicotinamide Phosphoribosyltransferase In Complex with the Specific Inhibitor FK-866
Authors : Kim, M.-K.; Eom, S.H.
Deposited on : 2006-03-05
Resolution : 2.90 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

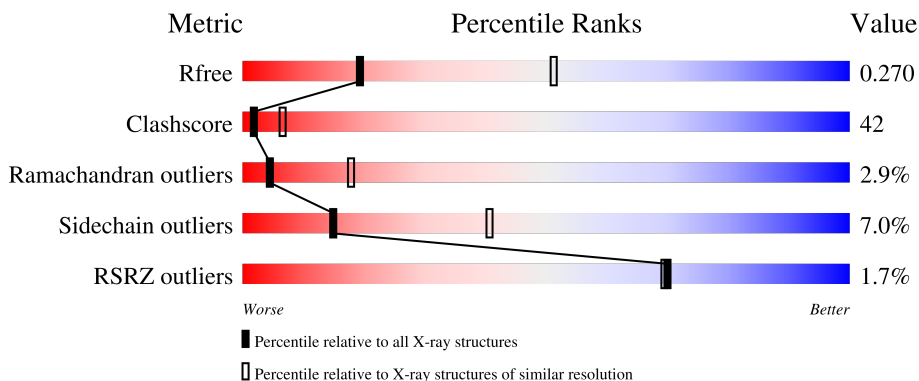
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	491	
1	B	491	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DGB	A	1001	-	-	X	-
2	DGB	B	1002	-	-	X	-

2 Entry composition [i](#)

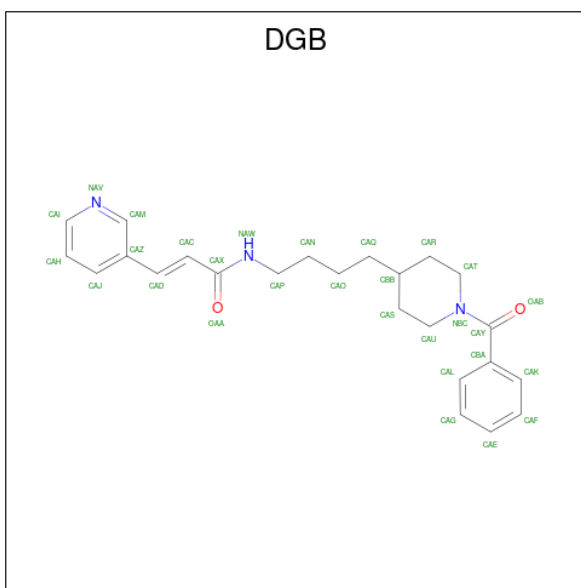
There are 3 unique types of molecules in this entry. The entry contains 7575 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nicotinamide phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	Total 3700	C 2374	N 616	O 704	S 6	0	0	0
1	B	463	Total 3700	C 2374	N 616	O 704	S 6	0	0	0

- Molecule 2 is (2E)-N-{4-[1-(benzenecarbonyl)piperidin-4-yl]butyl}-3-(pyridin-3-yl)prop-2-enamide (three-letter code: DGB) (formula: C₂₄H₂₉N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 29	C 24	N 3	O 2	0	0
2	B	1	Total 29	C 24	N 3	O 2	0	0

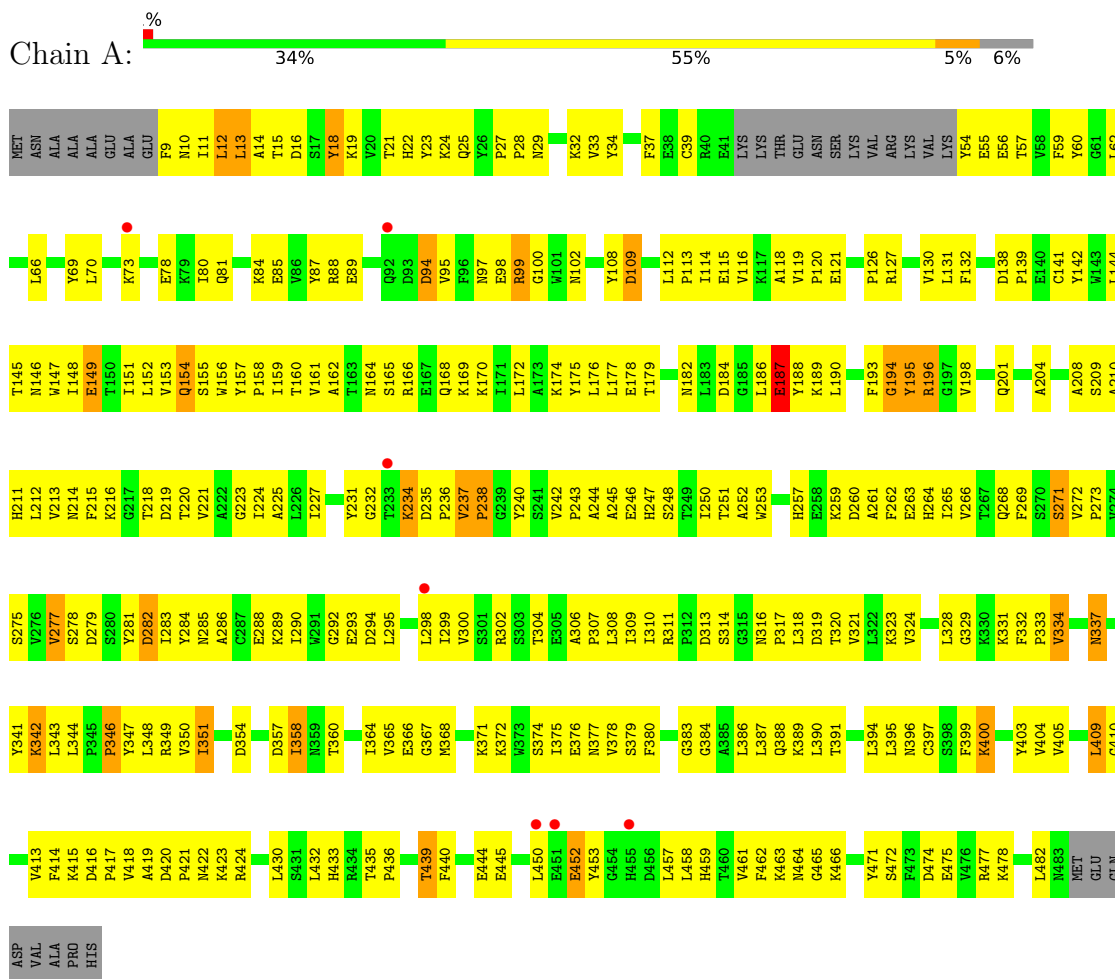
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	0	0
3	B	49	Total 49	O 49	0	0

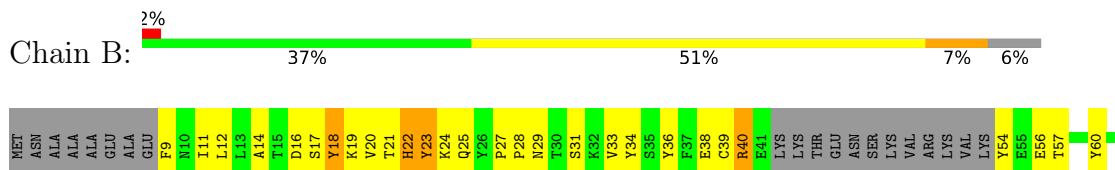
3 Residue-property plots [i](#)

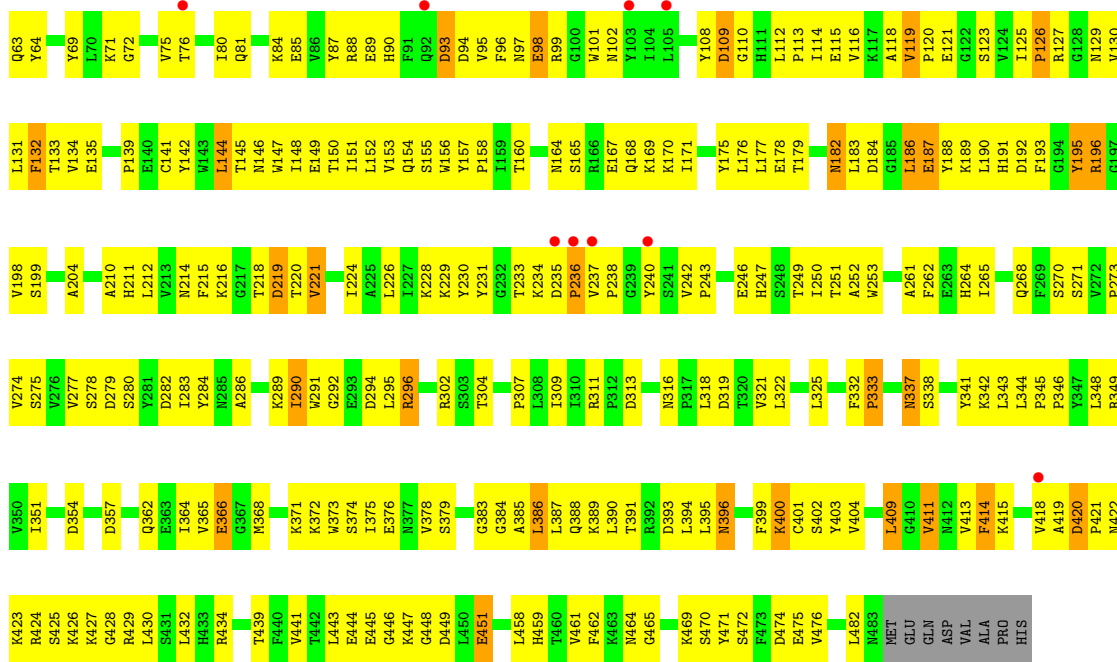
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Nicotinamide phosphoribosyltransferase



- Molecule 1: Nicotinamide phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 106.48Å 118.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 38.74 – 3.01	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.90) 92.4 (38.74-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.49 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.268 0.242 , 0.270	Depositor DCC
R_{free} test set	2049 reflections (9.84%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtrriage
Anisotropy	0.526	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7575	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 58.21 % 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 2.1136e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.39	0/3788	0.64	0/5136
1	B	0.38	0/3788	0.64	0/5136
All	All	0.38	0/7576	0.64	0/10272

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3700	0	3665	348	0
1	B	3700	0	3665	305	0
2	A	29	0	31	14	0
2	B	29	0	31	18	0
3	A	68	0	0	22	0
3	B	49	0	0	5	0
All	All	7575	0	7392	626	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 42.

All (626) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:HG22	1:B:390:LEU:HD23	1.39	1.03
1:A:272:VAL:HB	1:A:273:PRO:HD2	1.42	1.02
1:A:439:THR:HG22	1:A:440:PHE:H	1.27	0.99
1:B:116:VAL:HG22	1:B:134:VAL:HG22	1.46	0.97
1:A:413:VAL:HG21	1:B:252:ALA:HA	1.45	0.94
1:A:196:ARG:HG2	1:A:196:ARG:HH11	1.29	0.93
1:A:172:LEU:HD13	1:A:189:LYS:HB3	1.52	0.91
1:A:316:ASN:ND2	1:A:319:ASP:H	1.69	0.91
1:A:318:LEU:HD23	1:A:364:ILE:HA	1.53	0.91
1:B:286:ALA:HA	1:B:290:ILE:HG13	1.55	0.89
1:B:179:THR:CG2	1:B:374:SER:HA	2.03	0.88
1:B:196:ARG:NH2	2:B:1002:DGB:HAI	1.88	0.88
1:A:208:ALA:HB3	1:A:223:GLY:HA3	1.55	0.88
1:B:179:THR:HG21	1:B:374:SER:HA	1.57	0.87
1:A:145:THR:HG22	3:A:1027:HOH:O	1.75	0.86
1:B:149:GLU:HG3	1:B:399:PHE:CD2	2.11	0.86
1:A:432:LEU:HD12	1:A:457:LEU:HB2	1.59	0.83
1:A:242:VAL:HG11	2:A:1001:DGB:HAR2	1.61	0.82
1:B:273:PRO:HB3	1:B:307:PRO:HD2	1.58	0.82
1:B:175:TYR:OH	1:B:366:GLU:HG2	1.78	0.82
1:A:19:LYS:HA	1:A:22:HIS:CD2	2.16	0.81
1:B:171:ILE:HG12	1:B:362:GLN:NE2	1.95	0.80
1:B:11:ILE:HG23	1:B:12:LEU:HD23	1.61	0.80
1:A:250:ILE:HD12	1:A:277:VAL:HG23	1.64	0.79
1:A:11:ILE:H	1:A:11:ILE:HD12	1.47	0.78
1:A:295:LEU:HD12	1:A:298:LEU:HD12	1.64	0.78
1:A:459:HIS:O	1:A:461:VAL:HG13	1.84	0.78
1:B:34:TYR:HD2	1:B:403:TYR:HB3	1.49	0.77
1:B:237:VAL:HG11	1:B:240:TYR:HB2	1.65	0.77
1:A:244:ALA:HB2	1:A:275:SER:HB3	1.65	0.77
1:A:34:TYR:HB3	1:A:403:TYR:HB3	1.65	0.77
1:B:54:TYR:OH	1:B:164:ASN:ND2	2.18	0.76
2:A:1001:DGB:HAU2	2:A:1001:DGB:CAK	2.13	0.76
1:A:259:LYS:HG3	1:A:295:LEU:HD21	1.68	0.76
1:A:391:THR:HG21	1:B:389:LYS:HG2	1.68	0.76
1:B:19:LYS:HA	1:B:22:HIS:CG	2.21	0.76
1:A:21:THR:HG22	1:A:95:VAL:HG11	1.66	0.76
1:B:40:ARG:HB2	1:B:396:ASN:HB3	1.68	0.75
1:A:97:ASN:HD21	1:A:100:GLY:HA3	1.52	0.75
1:B:235:ASP:OD1	1:B:236:PRO:HD2	1.87	0.75
1:B:234:LYS:HD2	1:B:234:LYS:N	2.01	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:N	1:A:234:LYS:HD2	2.03	0.74
1:A:118:ALA:HA	1:A:458:LEU:HD22	1.68	0.74
1:A:88:ARG:NH1	1:A:94:ASP:HB2	2.02	0.73
1:B:193:PHE:CZ	2:B:1002:DGB:HAD1	2.23	0.73
1:B:415:LYS:H	1:B:425:SER:HB3	1.53	0.73
1:B:311:ARG:HB2	1:B:351:ILE:CG2	2.19	0.73
1:A:88:ARG:HH11	1:A:94:ASP:HB2	1.51	0.73
1:B:36:TYR:HE1	1:B:38:GLU:HG2	1.53	0.72
1:B:400:LYS:HE2	1:B:401:CYS:H	1.53	0.72
1:B:98:GLU:O	1:B:102:ASN:HB2	1.87	0.72
1:A:156:TRP:HH2	1:B:388:GLN:HE21	1.38	0.72
2:B:1002:DGB:HAU2	2:B:1002:DGB:CAK	2.19	0.72
1:A:244:ALA:CB	1:A:275:SER:HB3	2.20	0.72
1:A:318:LEU:HD21	1:A:367:GLY:HA3	1.71	0.71
1:A:311:ARG:HB2	1:A:351:ILE:HG13	1.73	0.71
1:B:34:TYR:CD2	1:B:403:TYR:HB3	2.26	0.71
1:A:13:LEU:HA	1:A:87:TYR:OH	1.91	0.71
1:A:33:VAL:HG11	1:A:142:TYR:O	1.90	0.71
1:A:182:ASN:HD22	1:A:184:ASP:H	1.38	0.71
1:B:112:LEU:HD22	1:B:144:LEU:HD11	1.72	0.71
1:A:351:ILE:HA	1:A:379:SER:O	1.91	0.70
1:B:286:ALA:HA	1:B:290:ILE:CG1	2.22	0.70
1:A:243:PRO:HB3	1:B:21:THR:HG21	1.74	0.70
1:B:196:ARG:NH2	2:B:1002:DGB:CAI	2.55	0.70
1:B:31:SER:O	1:B:139:PRO:HA	1.92	0.70
1:A:196:ARG:HH11	1:A:196:ARG:CG	2.05	0.69
1:A:309:ILE:HG22	1:A:351:ILE:HG12	1.75	0.69
1:A:272:VAL:HB	1:A:273:PRO:CD	2.20	0.69
1:B:182:ASN:ND2	1:B:184:ASP:H	1.90	0.69
1:A:472:SER:OG	1:A:475:GLU:HG3	1.92	0.69
1:B:148:ILE:O	1:B:151:ILE:HG22	1.93	0.69
1:A:9:PHE:CE2	1:A:69:TYR:HD2	2.12	0.68
1:A:198:VAL:HG21	1:A:204:ALA:HB2	1.75	0.68
1:B:81:GLN:O	1:B:85:GLU:HG3	1.94	0.68
1:A:247:HIS:HE1	1:A:279:ASP:OD2	1.77	0.68
1:B:278:SER:HB2	1:B:283:ILE:HD12	1.75	0.68
1:A:19:LYS:HA	1:A:22:HIS:CG	2.29	0.67
1:B:198:VAL:HG21	1:B:204:ALA:HB2	1.77	0.67
1:B:160:THR:CG2	1:B:390:LEU:HD23	2.22	0.67
1:B:21:THR:HG22	1:B:95:VAL:HG11	1.76	0.67
1:A:275:SER:OG	1:A:351:ILE:HD11	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ASN:HD22	1:B:184:ASP:H	1.39	0.67
1:B:311:ARG:NH2	2:B:1002:DGB:HAJ	2.09	0.67
1:B:57:THR:HG22	1:B:395:LEU:HD13	1.77	0.66
1:B:434:ARG:HG2	1:B:439:THR:O	1.95	0.66
1:A:311:ARG:CZ	2:A:1001:DGB:HAJ	2.26	0.66
1:A:179:THR:CG2	1:A:374:SER:HA	2.25	0.66
1:A:166:ARG:HG2	3:A:1038:HOH:O	1.96	0.66
1:A:212:LEU:HD21	1:A:218:THR:HB	1.78	0.66
1:A:430:LEU:CD2	1:A:444:GLU:HG2	2.26	0.66
1:A:21:THR:HG21	1:B:243:PRO:HB3	1.79	0.65
1:A:242:VAL:CG1	2:A:1001:DGB:HAR2	2.26	0.65
1:B:400:LYS:HE2	1:B:401:CYS:N	2.11	0.65
1:A:175:TYR:CE2	1:A:366:GLU:HG2	2.31	0.65
1:A:286:ALA:HA	1:A:290:ILE:CG1	2.26	0.65
1:B:192:ASP:HB2	1:B:211:HIS:ND1	2.10	0.65
1:A:349:ARG:HD2	2:A:1001:DGB:CAG	2.26	0.65
1:B:418:VAL:O	1:B:419:ALA:HB3	1.97	0.65
1:B:388:GLN:HG3	1:B:389:LYS:H	1.62	0.65
1:B:36:TYR:HE1	1:B:38:GLU:CG	2.10	0.65
1:A:439:THR:HG22	1:A:440:PHE:N	2.07	0.65
1:A:288:GLU:O	1:A:293:GLU:HG3	1.97	0.65
1:A:187:GLU:OE1	1:A:216:LYS:HE2	1.97	0.65
1:A:316:ASN:HD21	1:A:319:ASP:H	1.42	0.65
1:A:11:ILE:HD12	1:A:11:ILE:N	2.11	0.64
1:A:286:ALA:HA	1:A:290:ILE:HG12	1.80	0.64
1:A:450:LEU:HB2	1:A:452:GLU:HG3	1.79	0.64
1:B:151:ILE:CG2	1:B:152:LEU:N	2.61	0.64
1:A:365:VAL:HG13	1:A:375:ILE:HD12	1.80	0.64
1:B:311:ARG:HB2	1:B:351:ILE:HG23	1.78	0.64
1:B:54:TYR:HE1	1:B:394:LEU:HD11	1.61	0.64
1:B:343:LEU:HD12	1:B:344:LEU:N	2.13	0.63
1:B:196:ARG:HH21	2:B:1002:DGB:HAI	1.63	0.63
1:A:116:VAL:HB	1:A:462:PHE:HB3	1.80	0.63
1:A:169:LYS:HG2	1:A:482:LEU:HD11	1.80	0.63
1:A:209:SER:O	1:A:213:VAL:HG23	1.97	0.63
1:B:36:TYR:CE1	1:B:38:GLU:HG2	2.34	0.63
1:B:292:GLY:O	1:B:296:ARG:HG3	1.98	0.63
1:A:99:ARG:HH11	1:A:99:ARG:HB2	1.62	0.63
1:A:399:PHE:HE2	3:A:1027:HOH:O	1.82	0.62
1:A:236:PRO:HB2	1:B:89:GLU:OE1	1.99	0.62
1:A:277:VAL:HG13	1:A:311:ARG:NH1	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG13	1:A:375:ILE:CD1	2.28	0.62
1:B:270:SER:HA	1:B:302:ARG:HH12	1.62	0.62
1:A:27:PRO:HG3	1:B:253:TRP:CG	2.35	0.62
1:B:84:LYS:HA	1:B:96:PHE:CD2	2.33	0.62
1:A:10:ASN:OD1	1:A:12:LEU:N	2.33	0.62
1:B:113:PRO:HG3	1:B:141:CYS:SG	2.40	0.62
1:A:188:TYR:HE2	3:A:1008:HOH:O	1.83	0.61
1:A:208:ALA:HB3	1:A:223:GLY:CA	2.30	0.61
1:A:266:VAL:HG12	1:A:308:LEU:HD13	1.83	0.61
1:A:10:ASN:OD1	1:A:12:LEU:HB2	2.00	0.61
1:A:175:TYR:OH	1:A:366:GLU:HG2	2.00	0.61
1:A:329:GLY:HA2	1:A:334:VAL:HG13	1.81	0.61
1:B:333:PRO:O	1:B:345:PRO:HD3	2.00	0.61
1:B:56:GLU:HA	1:B:126:PRO:HA	1.83	0.61
1:B:134:VAL:HG12	1:B:145:THR:HG23	1.82	0.61
1:A:272:VAL:C	1:A:306:ALA:HB1	2.21	0.60
1:B:120:PRO:HG2	1:B:123:SER:OG	2.01	0.60
1:B:311:ARG:CZ	2:B:1002:DGB:HAJ	2.31	0.60
1:A:19:LYS:HG2	1:A:22:HIS:CD2	2.36	0.60
1:B:33:VAL:HB	3:B:1031:HOH:O	2.02	0.60
1:B:115:GLU:HA	1:B:462:PHE:O	2.02	0.60
1:B:40:ARG:CZ	1:B:423:LYS:HA	2.31	0.60
1:A:149:GLU:HB2	1:A:399:PHE:CD2	2.36	0.60
1:B:235:ASP:CG	1:B:236:PRO:HD2	2.21	0.60
1:A:54:TYR:HE1	1:A:394:LEU:HD11	1.67	0.60
1:B:325:LEU:HD11	1:B:368:MET:HE1	1.84	0.60
1:A:316:ASN:ND2	1:A:319:ASP:N	2.46	0.60
1:B:134:VAL:HG21	1:B:152:LEU:CD1	2.31	0.60
1:B:262:PHE:HE2	1:B:286:ALA:HB1	1.67	0.60
1:B:325:LEU:HD22	1:B:373:TRP:CE3	2.37	0.60
1:A:313:ASP:HB2	1:A:354:ASP:OD2	2.01	0.59
1:B:196:ARG:HG2	1:B:196:ARG:HH11	1.68	0.59
1:A:175:TYR:CD2	1:A:365:VAL:HG12	2.37	0.59
1:B:151:ILE:HG23	1:B:152:LEU:N	2.17	0.59
1:A:56:GLU:HA	1:A:126:PRO:HA	1.85	0.59
1:B:119:VAL:HG13	1:B:458:LEU:CD2	2.33	0.59
1:B:342:LYS:HD3	1:B:372:LYS:O	2.03	0.59
1:B:171:ILE:HG12	1:B:362:GLN:HE21	1.68	0.59
1:B:449:ASP:C	1:B:451:GLU:H	2.05	0.59
1:A:208:ALA:CB	1:A:223:GLY:HA3	2.31	0.59
1:A:157:TYR:HB3	1:A:158:PRO:CD	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:ASN:C	1:B:337:ASN:HD22	2.04	0.58
1:A:9:PHE:HE2	1:A:11:ILE:HG13	1.68	0.58
1:A:240:TYR:HD1	3:A:1008:HOH:O	1.85	0.58
1:B:165:SER:HB3	1:B:214:ASN:HD22	1.68	0.58
1:A:263:GLU:HG3	1:A:298:LEU:HD11	1.85	0.58
1:B:57:THR:CG2	1:B:395:LEU:HD13	2.32	0.58
1:A:242:VAL:HG22	2:A:1001:DGB:HAO2	1.85	0.58
1:B:430:LEU:CD2	1:B:444:GLU:HG2	2.33	0.58
1:A:170:LYS:HE3	3:A:1038:HOH:O	2.03	0.58
1:B:365:VAL:HG22	1:B:375:ILE:HD12	1.86	0.58
1:A:310:ILE:HD12	1:A:328:LEU:HD11	1.86	0.58
1:A:413:VAL:HG22	1:B:251:THR:O	2.03	0.58
1:B:313:ASP:OD1	1:B:354:ASP:HB2	2.03	0.58
1:A:174:LYS:O	1:A:178:GLU:HG2	2.04	0.57
1:B:261:ALA:O	1:B:265:ILE:HD13	2.03	0.57
1:A:25:GLN:HG2	1:B:265:ILE:HG13	1.85	0.57
1:B:28:PRO:O	1:B:29:ASN:HB2	2.03	0.57
1:A:237:VAL:CG2	1:B:89:GLU:HG2	2.34	0.57
1:A:304:THR:HG22	1:A:346:PRO:HB2	1.86	0.57
1:B:289:LYS:HB2	1:B:289:LYS:NZ	2.20	0.57
1:A:81:GLN:O	1:A:85:GLU:HG3	2.04	0.57
1:B:116:VAL:O	1:B:461:VAL:HG22	2.03	0.57
1:B:130:VAL:O	1:B:130:VAL:HG13	2.05	0.57
1:A:263:GLU:HG3	1:A:298:LEU:CD1	2.35	0.57
1:A:196:ARG:NH1	3:A:1011:HOH:O	2.36	0.57
1:B:34:TYR:CE2	1:B:429:ARG:HA	2.39	0.57
1:B:337:ASN:HD21	1:B:341:TYR:H	1.51	0.57
1:B:351:ILE:HA	1:B:379:SER:O	2.03	0.57
1:B:179:THR:HG23	1:B:341:TYR:CG	2.39	0.57
1:B:149:GLU:HG3	1:B:399:PHE:CG	2.39	0.57
1:B:362:GLN:O	1:B:366:GLU:HB2	2.05	0.57
1:A:212:LEU:HD21	1:A:218:THR:CG2	2.34	0.56
1:B:157:TYR:HB3	1:B:158:PRO:CD	2.35	0.56
1:A:11:ILE:H	1:A:11:ILE:CD1	2.17	0.56
1:A:23:TYR:CZ	1:A:24:LYS:HG3	2.40	0.56
1:B:182:ASN:O	1:B:183:LEU:HD23	2.05	0.56
1:A:224:ILE:HG12	1:A:238:PRO:HG2	1.88	0.56
1:A:337:ASN:HD21	1:A:341:TYR:H	1.52	0.56
1:A:89:GLU:OE2	1:B:238:PRO:HD2	2.06	0.56
1:A:235:ASP:HB3	1:A:236:PRO:HD2	1.88	0.56
1:A:188:TYR:CE2	3:A:1008:HOH:O	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ARG:HH21	2:B:1002:DGB:CAI	2.18	0.56
1:A:212:LEU:HA	1:A:215:PHE:O	2.06	0.55
1:A:290:ILE:HG22	1:A:295:LEU:HD23	1.87	0.55
1:A:432:LEU:CD1	1:A:457:LEU:HD12	2.37	0.55
1:A:57:THR:HG22	1:A:395:LEU:HD13	1.89	0.55
1:B:430:LEU:HD22	1:B:444:GLU:HG2	1.87	0.55
1:A:162:ALA:HA	1:A:210:ALA:O	2.07	0.55
1:B:19:LYS:HA	1:B:22:HIS:CD2	2.41	0.55
1:A:337:ASN:C	1:A:337:ASN:HD22	2.10	0.55
1:B:178:GLU:O	1:B:178:GLU:HG2	2.06	0.55
1:A:10:ASN:HB2	3:A:1055:HOH:O	2.06	0.55
1:A:179:THR:HG21	1:A:375:ILE:H	1.71	0.54
1:B:275:SER:CB	2:B:1002:DGB:HAP2	2.38	0.54
1:B:146:ASN:O	1:B:149:GLU:N	2.34	0.54
1:B:164:ASN:HB3	3:B:1026:HOH:O	2.07	0.54
1:A:175:TYR:OH	1:A:366:GLU:CG	2.55	0.54
1:A:293:GLU:HG2	1:A:331:LYS:HE3	1.90	0.54
1:A:435:THR:HB	1:A:436:PRO:HD2	1.90	0.54
1:B:233:THR:CG2	1:B:235:ASP:HB3	2.37	0.54
1:B:378:VAL:HG12	1:B:379:SER:N	2.21	0.54
1:A:195:TYR:CD1	1:A:220:THR:HA	2.43	0.54
1:A:316:ASN:HD22	1:A:319:ASP:H	1.51	0.54
1:B:112:LEU:O	1:B:464:ASN:HA	2.07	0.54
1:B:415:LYS:NZ	1:B:423:LYS:HD2	2.23	0.54
1:B:409:LEU:HG	1:B:409:LEU:O	2.08	0.54
1:A:195:TYR:OH	1:B:14:ALA:HA	2.08	0.54
1:B:54:TYR:CE1	1:B:394:LEU:HD11	2.42	0.54
1:B:88:ARG:HA	1:B:93:ASP:O	2.08	0.54
1:A:178:GLU:HB2	3:A:1041:HOH:O	2.07	0.53
1:A:294:ASP:HB2	1:A:295:LEU:HD22	1.89	0.53
1:A:212:LEU:HD21	1:A:218:THR:CB	2.39	0.53
1:A:153:VAL:C	1:A:155:SER:H	2.12	0.53
1:A:182:ASN:ND2	1:A:184:ASP:H	2.04	0.53
1:A:317:PRO:HB2	1:A:364:ILE:HD11	1.91	0.53
1:A:403:TYR:O	1:A:404:VAL:HG23	2.08	0.53
1:B:169:LYS:HE2	1:B:186:LEU:HD13	1.89	0.53
1:B:212:LEU:HD21	1:B:218:THR:CG2	2.38	0.53
1:B:34:TYR:HD1	1:B:135:GLU:HB3	1.73	0.53
1:B:409:LEU:HD11	1:B:411:VAL:HG12	1.89	0.53
1:A:33:VAL:O	1:A:33:VAL:HG13	2.09	0.53
1:A:151:ILE:HG22	3:A:1003:HOH:O	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:VAL:HG13	1:A:238:PRO:HD2	1.89	0.53
1:B:119:VAL:HG13	1:B:458:LEU:HD23	1.89	0.53
1:B:384:GLY:O	1:B:388:GLN:O	2.25	0.53
1:A:240:TYR:HA	1:B:90:HIS:HD2	1.72	0.53
1:A:311:ARG:HD2	3:A:1004:HOH:O	2.07	0.53
1:A:420:ASP:OD1	1:A:423:LYS:N	2.42	0.53
1:A:113:PRO:HG3	1:A:141:CYS:SG	2.48	0.53
1:B:114:ILE:HG23	1:B:144:LEU:HD13	1.89	0.53
1:A:179:THR:HG23	1:A:341:TYR:CG	2.43	0.53
1:B:296:ARG:HD2	1:B:332:PHE:CE2	2.43	0.53
1:A:175:TYR:HE2	1:A:366:GLU:HG2	1.74	0.53
1:B:148:ILE:O	1:B:152:LEU:HG	2.08	0.52
1:B:193:PHE:CE1	2:B:1002:DGB:HAD1	2.43	0.52
1:A:216:LYS:HG2	1:A:477:ARG:HH12	1.74	0.52
1:A:240:TYR:HA	1:B:90:HIS:CD2	2.44	0.52
1:A:28:PRO:O	1:A:29:ASN:HB2	2.08	0.52
1:A:316:ASN:HD22	1:A:319:ASP:N	2.06	0.52
1:A:375:ILE:HG22	1:A:375:ILE:O	2.09	0.52
1:A:121:GLU:OE1	1:A:231:TYR:HE2	1.92	0.52
1:B:348:LEU:O	1:B:349:ARG:NH1	2.43	0.52
1:B:445:GLU:OE1	1:B:447:LYS:HE3	2.09	0.52
1:A:416:ASP:OD1	1:A:424:ARG:HG2	2.10	0.52
1:A:298:LEU:O	1:A:302:ARG:HG3	2.10	0.52
1:A:175:TYR:HB3	1:A:375:ILE:HG13	1.93	0.51
1:A:277:VAL:HG13	1:A:311:ARG:CZ	2.39	0.51
1:A:349:ARG:HD2	2:A:1001:DGB:CAE	2.40	0.51
1:A:9:PHE:CZ	1:A:69:TYR:HD2	2.27	0.51
1:A:33:VAL:HG13	1:A:145:THR:CB	2.41	0.51
1:A:234:LYS:HD2	1:A:234:LYS:H	1.75	0.51
1:A:282:ASP:OD1	1:A:285:ASN:N	2.44	0.51
1:B:415:LYS:HG2	1:B:425:SER:HB2	1.93	0.51
1:A:175:TYR:CZ	1:A:366:GLU:HG2	2.46	0.51
1:A:432:LEU:HD11	1:A:440:PHE:HD2	1.76	0.51
1:A:179:THR:HG21	1:A:374:SER:HA	1.92	0.51
1:B:388:GLN:HG3	1:B:389:LYS:N	2.26	0.51
1:B:146:ASN:O	1:B:147:TRP:C	2.48	0.51
1:A:188:TYR:OH	1:A:216:LYS:HE3	2.11	0.51
1:A:193:PHE:O	1:A:195:TYR:N	2.44	0.51
1:A:318:LEU:CD2	1:A:364:ILE:HA	2.35	0.51
1:B:374:SER:C	1:B:376:GLU:H	2.13	0.51
1:B:459:HIS:O	1:B:461:VAL:HG13	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PHE:CZ	1:A:397:CYS:HB3	2.46	0.50
1:B:116:VAL:HG13	1:B:133:THR:O	2.11	0.50
1:A:263:GLU:OE1	1:A:295:LEU:HD11	2.11	0.50
1:A:298:LEU:HD22	3:A:1060:HOH:O	2.11	0.50
1:B:40:ARG:NE	1:B:422:ASN:O	2.45	0.50
1:B:168:GLN:HA	1:B:171:ILE:HD12	1.92	0.50
1:B:294:ASP:O	1:B:295:LEU:HD23	2.11	0.50
1:B:415:LYS:HZ1	1:B:423:LYS:HD2	1.76	0.50
1:B:125:ILE:O	1:B:126:PRO:O	2.29	0.50
1:B:472:SER:OG	1:B:475:GLU:HG3	2.11	0.50
1:A:57:THR:CG2	1:A:395:LEU:HD13	2.42	0.50
1:A:149:GLU:O	1:A:153:VAL:HG23	2.12	0.50
1:A:351:ILE:HG22	1:A:379:SER:O	2.12	0.50
1:B:134:VAL:HG21	1:B:152:LEU:HD11	1.93	0.50
1:A:84:LYS:HD3	1:A:98:GLU:OE1	2.12	0.50
1:A:304:THR:HG23	3:A:1069:HOH:O	2.11	0.50
1:A:27:PRO:HG3	1:B:253:TRP:CD1	2.46	0.49
1:A:161:VAL:HB	1:A:210:ALA:CB	2.42	0.49
1:A:292:GLY:O	1:A:293:GLU:HG2	2.12	0.49
1:B:116:VAL:CG2	1:B:134:VAL:HG22	2.31	0.49
1:B:229:LYS:HD3	1:B:230:TYR:CE1	2.47	0.49
1:A:115:GLU:HG3	1:A:463:LYS:HD2	1.93	0.49
1:A:409:LEU:HD12	1:A:409:LEU:O	2.12	0.49
1:A:236:PRO:O	1:A:237:VAL:HB	2.11	0.49
1:A:245:ALA:HB2	1:A:265:ILE:HD13	1.93	0.49
1:B:318:LEU:HD23	1:B:318:LEU:O	2.12	0.49
1:A:273:PRO:HB3	1:A:307:PRO:HD2	1.95	0.49
1:A:251:THR:O	1:B:413:VAL:HG22	2.12	0.49
1:B:262:PHE:CD2	1:B:290:ILE:HG21	2.48	0.49
1:A:112:LEU:HD22	1:A:144:LEU:HD11	1.95	0.49
1:A:418:VAL:HG13	1:A:419:ALA:N	2.27	0.49
1:B:224:ILE:HG22	1:B:228:LYS:HE2	1.95	0.49
1:B:231:TYR:O	1:B:472:SER:HA	2.12	0.49
1:B:283:ILE:HG23	1:B:284:TYR:N	2.26	0.49
1:A:311:ARG:HB2	1:A:351:ILE:CG1	2.41	0.49
1:A:413:VAL:HG13	1:B:251:THR:HB	1.94	0.49
1:A:253:TRP:CG	1:B:27:PRO:HG3	2.48	0.49
1:A:317:PRO:HB2	1:A:364:ILE:CD1	2.42	0.49
1:B:118:ALA:HB2	1:B:132:PHE:HB2	1.95	0.49
1:B:176:LEU:CD1	1:B:189:LYS:HE3	2.43	0.49
1:B:374:SER:C	1:B:376:GLU:N	2.66	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:O	3:A:1008:HOH:O	2.20	0.49
1:A:415:LYS:HD2	1:B:247:HIS:ND1	2.28	0.49
1:B:349:ARG:HD2	2:B:1002:DGB:CAE	2.42	0.49
1:A:244:ALA:CB	2:A:1001:DGB:OAA	2.61	0.48
1:A:176:LEU:HD22	1:A:182:ASN:O	2.12	0.48
1:A:194:GLY:N	1:A:383:GLY:HA2	2.28	0.48
1:A:269:PHE:C	1:A:271:SER:N	2.63	0.48
1:B:64:TYR:CE1	1:B:226:LEU:HD11	2.49	0.48
1:B:449:ASP:C	1:B:451:GLU:N	2.66	0.48
1:A:130:VAL:O	1:A:130:VAL:HG13	2.13	0.48
1:B:167:GLU:O	1:B:171:ILE:HD12	2.13	0.48
1:B:278:SER:HB2	1:B:283:ILE:CD1	2.40	0.48
1:B:309:ILE:HG22	1:B:351:ILE:HG22	1.94	0.48
1:B:443:LEU:HD12	1:B:448:GLY:HA2	1.96	0.48
1:A:121:GLU:OE1	1:A:231:TYR:CE2	2.65	0.48
1:A:421:PRO:O	1:A:424:ARG:HG3	2.13	0.48
1:B:378:VAL:CG1	1:B:379:SER:N	2.76	0.48
1:A:62:LEU:HD11	1:A:66:LEU:HD21	1.96	0.48
1:B:318:LEU:HD23	1:B:322:LEU:HG	1.96	0.48
1:A:21:THR:HG21	1:B:243:PRO:CB	2.43	0.48
1:A:189:LYS:O	1:A:380:PHE:N	2.44	0.48
1:A:262:PHE:CD2	1:A:290:ILE:HG21	2.49	0.48
1:B:441:VAL:HG13	1:B:441:VAL:O	2.14	0.48
1:A:309:ILE:CG2	1:A:351:ILE:HG12	2.43	0.48
1:A:98:GLU:O	1:A:102:ASN:HB2	2.14	0.47
1:B:386:LEU:O	1:B:386:LEU:HD22	2.14	0.47
1:A:417:PRO:HG2	1:A:420:ASP:O	2.15	0.47
1:B:429:ARG:NH1	1:B:446:GLY:HA3	2.29	0.47
1:B:462:PHE:CZ	1:B:465:GLY:HA2	2.50	0.47
1:A:161:VAL:HB	1:A:210:ALA:HB3	1.95	0.47
1:A:278:SER:O	1:A:283:ILE:HA	2.14	0.47
1:A:415:LYS:NZ	1:B:247:HIS:CE1	2.82	0.47
1:B:191:HIS:HE1	1:B:219:ASP:OD1	1.98	0.47
1:A:212:LEU:HD12	1:A:227:ILE:HD12	1.97	0.47
1:A:300:VAL:HA	1:A:347:TYR:CE2	2.49	0.47
1:B:176:LEU:HD12	1:B:189:LYS:HE3	1.96	0.47
1:A:118:ALA:HB2	1:A:132:PHE:HB2	1.96	0.47
1:A:343:LEU:HD12	1:A:344:LEU:N	2.29	0.47
1:A:416:ASP:CG	1:A:424:ARG:HG2	2.34	0.47
1:A:430:LEU:HD23	1:A:444:GLU:HA	1.95	0.47
1:B:76:THR:O	1:B:80:ILE:HG13	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:O	1:A:404:VAL:HA	2.14	0.47
1:A:156:TRP:CH2	1:B:388:GLN:NE2	2.82	0.47
1:A:236:PRO:HG2	1:A:240:TYR:OH	2.15	0.47
1:B:16:ASP:HB2	1:B:19:LYS:HD2	1.96	0.47
1:B:270:SER:HA	1:B:302:ARG:NH1	2.28	0.47
1:A:246:GLU:OE2	1:B:146:ASN:ND2	2.46	0.47
1:B:242:VAL:CG1	2:B:1002:DGB:HAR2	2.45	0.47
1:B:274:VAL:HG13	1:B:274:VAL:O	2.15	0.47
1:A:146:ASN:CG	3:A:1027:HOH:O	2.53	0.47
1:A:156:TRP:HH2	1:B:388:GLN:NE2	2.09	0.47
1:B:18:TYR:CE2	1:B:19:LYS:HG3	2.49	0.47
1:B:409:LEU:CD1	1:B:411:VAL:HG12	2.45	0.47
1:A:9:PHE:CE2	1:A:11:ILE:HG13	2.49	0.47
1:B:175:TYR:CE2	1:B:366:GLU:HA	2.50	0.46
1:B:318:LEU:HD23	1:B:318:LEU:C	2.36	0.46
1:B:322:LEU:HD13	1:B:371:LYS:HG3	1.96	0.46
1:A:33:VAL:HG13	1:A:145:THR:HB	1.96	0.46
1:A:153:VAL:O	1:A:155:SER:N	2.48	0.46
1:A:240:TYR:HB2	3:A:1008:HOH:O	2.15	0.46
1:A:374:SER:C	1:A:376:GLU:H	2.18	0.46
1:A:97:ASN:ND2	1:A:100:GLY:HA3	2.27	0.46
2:A:1001:DGB:HAD1	3:A:1004:HOH:O	2.14	0.46
1:B:126:PRO:HG2	1:B:129:ASN:ND2	2.31	0.46
1:A:175:TYR:CG	1:A:365:VAL:HG12	2.51	0.46
1:A:211:HIS:C	1:A:213:VAL:H	2.17	0.46
1:A:300:VAL:HA	1:A:347:TYR:CZ	2.51	0.46
1:A:212:LEU:HD12	1:A:227:ILE:CD1	2.46	0.46
1:A:462:PHE:CZ	1:A:465:GLY:HA2	2.51	0.46
1:B:175:TYR:CG	1:B:365:VAL:CG1	2.98	0.46
1:B:177:LEU:HB2	1:B:183:LEU:HD21	1.97	0.46
1:B:318:LEU:HG	1:B:364:ILE:HA	1.98	0.46
1:A:78:GLU:H	1:A:78:GLU:CD	2.19	0.46
1:A:165:SER:HB3	1:A:214:ASN:HD22	1.80	0.46
1:A:332:PHE:HB3	1:A:333:PRO:HD2	1.97	0.46
1:B:196:ARG:HG2	1:B:196:ARG:NH1	2.31	0.46
1:B:337:ASN:ND2	1:B:341:TYR:H	2.14	0.46
1:A:16:ASP:OD1	1:B:195:TYR:HB3	2.16	0.46
1:A:114:ILE:HD13	1:A:148:ILE:CD1	2.46	0.46
1:A:154:GLN:NE2	1:B:198:VAL:HG23	2.30	0.46
1:A:237:VAL:HG23	1:B:89:GLU:HG2	1.98	0.46
1:A:295:LEU:HD22	1:A:295:LEU:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:HD13	1:B:148:ILE:CD1	2.46	0.46
1:A:144:LEU:O	1:A:147:TRP:HB3	2.15	0.46
1:B:316:ASN:HB3	1:B:319:ASP:HB2	1.98	0.46
1:A:62:LEU:O	1:A:66:LEU:HG	2.16	0.45
2:A:1001:DGB:CAK	2:A:1001:DGB:CAU	2.89	0.45
1:B:311:ARG:CB	1:B:351:ILE:HG23	2.44	0.45
1:B:449:ASP:O	1:B:451:GLU:HG3	2.15	0.45
1:A:208:ALA:O	1:A:212:LEU:HG	2.17	0.45
1:B:16:ASP:HB2	1:B:18:TYR:HE2	1.81	0.45
1:B:426:LYS:HD2	1:B:430:LEU:HD13	1.98	0.45
1:A:108:TYR:O	1:A:109:ASP:C	2.54	0.45
1:A:175:TYR:CG	1:A:365:VAL:CG1	3.00	0.45
1:A:211:HIS:CD2	1:A:386:LEU:HD21	2.52	0.45
1:A:223:GLY:O	1:A:227:ILE:HG13	2.15	0.45
1:A:284:TYR:CE2	1:A:323:LYS:HD3	2.51	0.45
1:B:34:TYR:HE2	1:B:429:ARG:HA	1.81	0.45
1:B:63:GLN:CD	1:B:470:SER:HB2	2.36	0.45
1:A:112:LEU:O	1:A:464:ASN:HA	2.16	0.45
1:A:320:THR:O	1:A:324:VAL:HG23	2.17	0.45
1:A:405:VAL:HA	1:A:410:GLY:HA2	1.98	0.45
1:B:418:VAL:O	1:B:419:ALA:CB	2.62	0.45
1:B:472:SER:C	1:B:474:ASP:N	2.70	0.45
1:B:199:SER:HB3	1:B:388:GLN:HE22	1.81	0.45
1:B:233:THR:HG22	1:B:235:ASP:N	2.32	0.45
1:A:244:ALA:HB3	2:A:1001:DGB:OAA	2.17	0.45
1:B:39:CYS:O	1:B:127:ARG:HG3	2.17	0.45
2:B:1002:DGB:CAK	2:B:1002:DGB:CAU	2.93	0.45
1:A:299:ILE:CD1	1:A:308:LEU:HD22	2.47	0.45
1:B:153:VAL:C	1:B:155:SER:H	2.21	0.45
1:B:191:HIS:ND1	1:B:193:PHE:HE2	2.15	0.45
1:A:13:LEU:HB2	1:B:221:VAL:HG11	1.98	0.44
1:A:33:VAL:HG13	1:A:145:THR:OG1	2.17	0.44
1:A:310:ILE:HD12	1:A:328:LEU:CD1	2.47	0.44
1:A:343:LEU:HD12	1:A:377:ASN:OD1	2.16	0.44
1:A:388:GLN:O	1:A:389:LYS:HB3	2.17	0.44
1:B:246:GLU:HG2	1:B:249:THR:HG23	1.98	0.44
1:A:253:TRP:CD1	1:B:27:PRO:HG3	2.52	0.44
1:B:22:HIS:HA	1:B:25:GLN:HE21	1.81	0.44
1:A:453:TYR:CD1	1:A:453:TYR:N	2.85	0.44
1:B:112:LEU:CD2	1:B:144:LEU:HD11	2.44	0.44
1:A:16:ASP:HB2	1:A:18:TYR:HE2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:VAL:CG2	2:A:1001:DGB:HAO2	2.46	0.44
1:A:144:LEU:O	1:A:144:LEU:HD23	2.18	0.44
1:B:120:PRO:HB3	1:B:471:TYR:CE2	2.53	0.44
1:B:459:HIS:CD2	1:B:469:LYS:NZ	2.86	0.44
1:A:55:GLU:O	1:A:126:PRO:HA	2.17	0.44
2:A:1001:DGB:CAD	3:A:1004:HOH:O	2.66	0.44
1:B:22:HIS:O	1:B:24:LYS:N	2.51	0.44
1:B:188:TYR:HE2	1:B:240:TYR:HB3	1.81	0.44
1:A:357:ASP:C	1:A:357:ASP:OD2	2.56	0.44
1:B:132:PHE:CD1	1:B:132:PHE:C	2.90	0.44
1:A:60:TYR:H	1:A:159:ILE:HG12	1.83	0.44
1:B:421:PRO:CB	1:B:424:ARG:HH21	2.30	0.44
1:A:252:ALA:HA	1:B:413:VAL:HG21	2.00	0.43
1:A:281:TYR:O	1:A:282:ASP:C	2.55	0.43
1:B:430:LEU:HA	1:B:443:LEU:O	2.18	0.43
1:A:19:LYS:C	1:A:21:THR:N	2.70	0.43
1:A:39:CYS:HB3	1:A:395:LEU:O	2.19	0.43
1:A:119:VAL:HG22	1:A:131:LEU:O	2.18	0.43
1:A:318:LEU:HD13	1:A:318:LEU:C	2.38	0.43
1:A:384:GLY:O	1:A:388:GLN:N	2.38	0.43
1:B:121:GLU:HB2	1:B:476:VAL:HG22	1.99	0.43
1:B:357:ASP:OD2	1:B:357:ASP:C	2.57	0.43
1:B:242:VAL:HG22	2:B:1002:DGB:HAN1	1.99	0.43
1:A:224:ILE:HG23	1:A:238:PRO:CG	2.48	0.43
1:A:351:ILE:HD13	2:A:1001:DGB:HAP2	2.00	0.43
1:B:278:SER:O	1:B:283:ILE:HA	2.18	0.43
1:B:325:LEU:HB3	1:B:373:TRP:CZ2	2.53	0.43
1:B:402:SER:O	1:B:428:GLY:N	2.47	0.43
1:A:33:VAL:CG1	1:A:142:TYR:O	2.63	0.43
1:A:59:PHE:CD1	1:A:131:LEU:HB3	2.53	0.43
1:A:170:LYS:HD3	3:A:1014:HOH:O	2.18	0.43
1:A:478:LYS:HA	3:A:1054:HOH:O	2.18	0.43
1:B:75:VAL:HB	1:B:110:GLY:HA2	2.01	0.43
1:A:351:ILE:HG23	1:A:379:SER:OG	2.18	0.43
1:A:391:THR:CG2	1:B:389:LYS:HG2	2.43	0.43
1:B:108:TYR:O	1:B:109:ASP:C	2.57	0.43
1:B:386:LEU:HD13	1:B:387:LEU:CD2	2.49	0.43
1:A:54:TYR:OH	1:A:164:ASN:ND2	2.51	0.43
1:A:201:GLN:O	1:A:204:ALA:HB3	2.19	0.43
1:A:253:TRP:CD1	1:A:261:ALA:HB2	2.53	0.43
1:A:329:GLY:HA2	1:A:334:VAL:CG1	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:CYS:O	1:B:40:ARG:C	2.56	0.43
1:B:71:LYS:CG	1:B:72:GLY:N	2.82	0.43
1:B:429:ARG:NH2	1:B:449:ASP:OD2	2.48	0.43
1:A:304:THR:CG2	1:A:346:PRO:HB2	2.49	0.43
1:A:415:LYS:NZ	1:B:247:HIS:HE1	2.17	0.43
1:B:296:ARG:HD2	1:B:332:PHE:CZ	2.53	0.43
1:B:351:ILE:HG23	1:B:351:ILE:O	2.19	0.43
1:A:9:PHE:CZ	1:A:69:TYR:CD2	3.06	0.43
1:A:198:VAL:HG12	1:A:387:LEU:HB3	2.00	0.43
1:A:310:ILE:CD1	1:A:348:LEU:HD11	2.49	0.43
1:A:342:LYS:HZ2	1:A:342:LYS:CB	2.31	0.43
1:A:413:VAL:CG1	1:A:414:PHE:N	2.82	0.43
1:B:12:LEU:HD12	1:B:80:ILE:HA	2.00	0.43
1:B:71:LYS:HG2	1:B:72:GLY:N	2.34	0.43
1:B:186:LEU:C	1:B:188:TYR:H	2.22	0.43
1:B:264:HIS:O	1:B:268:GLN:HG2	2.19	0.43
1:B:389:LYS:C	1:B:390:LEU:HD12	2.39	0.43
1:A:15:THR:OG1	1:A:19:LYS:HD2	2.18	0.42
1:A:114:ILE:O	1:A:463:LYS:HA	2.19	0.42
1:A:119:VAL:HG13	1:A:458:LEU:HD23	2.00	0.42
1:A:120:PRO:HB3	1:A:471:TYR:CE2	2.54	0.42
1:A:221:VAL:HG11	1:B:87:TYR:HE2	1.84	0.42
1:A:266:VAL:CG1	1:A:308:LEU:HD13	2.48	0.42
1:A:432:LEU:HD13	1:A:432:LEU:C	2.40	0.42
1:A:211:HIS:C	1:A:213:VAL:N	2.73	0.42
1:A:262:PHE:HE2	1:A:286:ALA:HB1	1.84	0.42
1:A:278:SER:O	1:A:283:ILE:HD12	2.19	0.42
1:A:415:LYS:HZ2	1:B:247:HIS:CE1	2.38	0.42
1:B:95:VAL:HG12	1:B:95:VAL:O	2.20	0.42
1:B:165:SER:OG	1:B:211:HIS:CD2	2.72	0.42
1:A:196:ARG:HG2	1:A:196:ARG:NH1	2.09	0.42
1:A:371:LYS:O	1:A:372:LYS:HB2	2.20	0.42
1:B:153:VAL:O	1:B:155:SER:N	2.52	0.42
1:B:385:ALA:O	1:B:390:LEU:HD11	2.19	0.42
1:B:420:ASP:C	1:B:422:ASN:H	2.23	0.42
1:A:23:TYR:CE1	1:A:24:LYS:HG3	2.54	0.42
1:A:151:ILE:HG23	1:A:152:LEU:N	2.34	0.42
1:A:273:PRO:HB3	1:A:306:ALA:HA	2.01	0.42
1:A:289:LYS:HE3	1:A:289:LYS:HB2	1.66	0.42
1:B:33:VAL:HB	1:B:142:TYR:O	2.19	0.42
1:B:120:PRO:HA	1:B:471:TYR:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:CB	1:A:403:TYR:HB3	2.44	0.42
1:A:286:ALA:HA	1:A:290:ILE:HG13	2.00	0.42
1:B:148:ILE:HB	1:B:151:ILE:HG22	2.01	0.42
1:B:195:TYR:CG	1:B:220:THR:HG23	2.55	0.42
1:B:278:SER:HA	3:B:1003:HOH:O	2.18	0.42
1:A:250:ILE:CD1	1:A:277:VAL:HG23	2.41	0.42
1:A:343:LEU:HD12	1:A:344:LEU:H	1.84	0.42
1:A:364:ILE:HG22	1:A:368:MET:HE2	2.00	0.42
1:A:453:TYR:H	1:A:453:TYR:HD1	1.68	0.42
1:B:304:THR:HG22	1:B:346:PRO:HB2	2.02	0.42
1:B:337:ASN:C	1:B:337:ASN:ND2	2.73	0.42
1:B:17:SER:OG	1:B:90:HIS:HE1	2.03	0.42
1:B:156:TRP:CD2	1:B:157:TYR:N	2.88	0.42
1:A:54:TYR:CE1	1:A:394:LEU:HD11	2.53	0.42
1:B:16:ASP:HB2	1:B:18:TYR:CE2	2.55	0.42
1:B:325:LEU:HD11	1:B:368:MET:CE	2.49	0.42
1:B:413:VAL:CG1	1:B:414:PHE:N	2.83	0.42
1:A:120:PRO:HA	1:A:471:TYR:CZ	2.55	0.41
1:A:145:THR:O	1:A:148:ILE:HG12	2.20	0.41
1:A:172:LEU:O	1:A:176:LEU:HB2	2.20	0.41
1:A:246:GLU:HG3	1:A:248:SER:H	1.83	0.41
1:B:23:TYR:CE2	1:B:97:ASN:HB2	2.55	0.41
1:B:31:SER:HB2	1:B:139:PRO:CB	2.50	0.41
1:B:427:LYS:O	1:B:444:GLU:HB3	2.19	0.41
1:A:257:HIS:ND1	1:A:260:ASP:OD2	2.47	0.41
1:A:388:GLN:HG3	1:A:389:LYS:H	1.85	0.41
1:B:17:SER:O	1:B:20:VAL:HG23	2.21	0.41
1:B:279:ASP:O	1:B:280:SER:C	2.58	0.41
1:A:27:PRO:HA	1:A:28:PRO:HD3	1.97	0.41
1:A:151:ILE:HG23	1:A:152:LEU:H	1.86	0.41
1:A:432:LEU:HD13	1:A:433:HIS:N	2.35	0.41
1:B:12:LEU:HD22	1:B:101:TRP:CZ2	2.55	0.41
1:B:236:PRO:HG2	1:B:237:VAL:H	1.84	0.41
2:B:1002:DGB:OAA	2:B:1002:DGB:CAN	2.68	0.41
1:A:73:LYS:HG3	1:A:109:ASP:O	2.20	0.41
1:A:168:GLN:HG2	1:A:358:ILE:HA	2.03	0.41
1:A:224:ILE:O	1:A:225:ALA:C	2.59	0.41
1:A:264:HIS:O	1:A:268:GLN:HG2	2.19	0.41
1:A:160:THR:O	1:A:161:VAL:C	2.58	0.41
1:B:31:SER:HB2	1:B:139:PRO:HB3	2.02	0.41
1:B:168:GLN:HA	1:B:171:ILE:CD1	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:SER:HB2	3:B:1041:HOH:O	2.20	0.41
1:B:289:LYS:HB2	1:B:289:LYS:HZ3	1.86	0.41
1:A:14:ALA:HA	3:B:1029:HOH:O	2.20	0.41
1:A:132:PHE:CD1	1:A:132:PHE:C	2.93	0.41
1:A:310:ILE:HB	1:A:350:VAL:HG22	2.02	0.41
1:A:400:LYS:HE3	1:A:415:LYS:HD3	2.02	0.41
1:B:304:THR:CG2	1:B:346:PRO:HB2	2.51	0.41
1:B:391:THR:C	1:B:393:ASP:N	2.72	0.41
1:A:182:ASN:ND2	1:A:184:ASP:CG	2.73	0.41
1:A:212:LEU:HD21	1:A:218:THR:HG21	2.01	0.41
1:B:187:GLU:OE1	1:B:216:LYS:HD2	2.21	0.41
1:B:212:LEU:HD21	1:B:218:THR:HG21	2.01	0.41
1:A:153:VAL:C	1:A:155:SER:N	2.73	0.41
1:A:157:TYR:HB3	1:A:158:PRO:HD3	2.03	0.41
1:B:321:VAL:O	1:B:325:LEU:HD12	2.21	0.41
1:B:343:LEU:HD12	1:B:343:LEU:C	2.41	0.41
1:B:60:TYR:CE2	1:B:210:ALA:HA	2.55	0.41
1:B:167:GLU:O	1:B:170:LYS:HB2	2.20	0.41
1:B:283:ILE:CG2	1:B:284:TYR:N	2.84	0.41
1:B:286:ALA:O	1:B:291:TRP:CD1	2.74	0.41
1:B:415:LYS:NZ	1:B:423:LYS:CD	2.84	0.41
1:A:378:VAL:HB	3:A:1063:HOH:O	2.20	0.41
1:B:148:ILE:HB	1:B:151:ILE:CG2	2.51	0.41
1:A:195:TYR:O	1:A:195:TYR:HD2	2.04	0.40
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.70	0.40
1:A:212:LEU:HD13	1:A:238:PRO:HB2	2.02	0.40
1:A:368:MET:HE3	1:A:380:PHE:HZ	1.86	0.40
1:B:9:PHE:CE2	1:B:69:TYR:CD2	3.09	0.40
1:B:119:VAL:HG22	1:B:131:LEU:O	2.21	0.40
1:A:62:LEU:HG	1:A:66:LEU:HD11	2.03	0.40
1:A:80:ILE:HG22	1:A:98:GLU:HG3	2.03	0.40
1:A:300:VAL:HG13	1:A:347:TYR:CE2	2.56	0.40
1:B:169:LYS:HD3	1:B:482:LEU:HD11	2.03	0.40
1:A:290:ILE:HG12	1:A:290:ILE:H	1.71	0.40
1:A:430:LEU:HD21	1:A:444:GLU:HG2	2.03	0.40
1:B:169:LYS:HA	1:B:215:PHE:HZ	1.86	0.40
1:B:311:ARG:HG3	1:B:351:ILE:HG23	2.03	0.40
1:B:419:ALA:O	1:B:420:ASP:HB2	2.21	0.40
2:B:1002:DGB:OAA	2:B:1002:DGB:HAN2	2.21	0.40
1:A:18:TYR:OH	1:B:196:ARG:NH2	2.54	0.40
1:A:138:ASP:HA	1:A:139:PRO:HD2	1.76	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PRO:O	1:A:321:VAL:HG23	2.22	0.40
1:A:364:ILE:H	1:A:364:ILE:HG13	1.70	0.40
1:A:466:LYS:HA	1:A:466:LYS:HD3	1.93	0.40
1:B:16:ASP:CB	1:B:18:TYR:HE2	2.34	0.40
1:B:33:VAL:HA	1:B:404:VAL:HG22	2.03	0.40
1:B:275:SER:HB3	2:B:1002:DGB:HAP2	2.03	0.40
1:B:342:LYS:HE2	1:B:373:TRP:CH2	2.57	0.40
1:A:177:LEU:HD12	1:A:182:ASN:HA	2.04	0.40
1:B:23:TYR:CZ	1:B:97:ASN:HB2	2.56	0.40
1:B:250:ILE:HD13	1:B:262:PHE:HE1	1.87	0.40
1:B:379:SER:HB3	2:B:1002:DGB:CAF	2.51	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	459/491 (94%)	383 (83%)	62 (14%)	14 (3%)	4 16
1	B	459/491 (94%)	397 (86%)	49 (11%)	13 (3%)	5 19
All	All	918/982 (94%)	780 (85%)	111 (12%)	27 (3%)	4 18

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	282	ASP
1	A	154	GLN
1	A	194	GLY
1	A	271	SER
1	A	282	ASP
1	A	445	GLU
1	B	126	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	187	GLU
1	A	187	GLU
1	A	232	GLY
1	A	238	PRO
1	A	439	THR
1	A	452	GLU
1	B	23	TYR
1	B	40	ARG
1	B	109	ASP
1	A	109	ASP
1	A	346	PRO
1	B	154	GLN
1	B	236	PRO
1	B	420	ASP
1	B	451	GLU
1	A	237	VAL
1	A	358	ILE
1	B	333	PRO
1	B	221	VAL
1	B	383	GLY

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	408/431 (95%)	380 (93%)	28 (7%)	15	41
1	B	408/431 (95%)	379 (93%)	29 (7%)	14	40
All	All	816/862 (95%)	759 (93%)	57 (7%)	15	41

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	LEU
1	A	18	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	70	LEU
1	A	94	ASP
1	A	99	ARG
1	A	127	ARG
1	A	149	GLU
1	A	186	LEU
1	A	187	GLU
1	A	190	LEU
1	A	195	TYR
1	A	196	ARG
1	A	219	ASP
1	A	234	LYS
1	A	277	VAL
1	A	314	SER
1	A	334	VAL
1	A	337	ASN
1	A	342	LYS
1	A	351	ILE
1	A	360	THR
1	A	390	LEU
1	A	396	ASN
1	A	400	LYS
1	A	409	LEU
1	A	422	ASN
1	A	474	ASP
1	B	18	TYR
1	B	22	HIS
1	B	93	ASP
1	B	94	ASP
1	B	98	GLU
1	B	99	ARG
1	B	119	VAL
1	B	132	PHE
1	B	144	LEU
1	B	150	THR
1	B	182	ASN
1	B	186	LEU
1	B	190	LEU
1	B	195	TYR
1	B	196	ARG
1	B	219	ASP
1	B	277	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	290	ILE
1	B	296	ARG
1	B	337	ASN
1	B	338	SER
1	B	366	GLU
1	B	386	LEU
1	B	396	ASN
1	B	400	LYS
1	B	409	LEU
1	B	411	VAL
1	B	414	PHE
1	B	432	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	90	HIS
1	A	97	ASN
1	A	111	HIS
1	A	164	ASN
1	A	168	GLN
1	A	182	ASN
1	A	211	HIS
1	A	214	ASN
1	A	247	HIS
1	A	285	ASN
1	A	316	ASN
1	A	337	ASN
1	A	388	GLN
1	A	396	ASN
1	A	422	ASN
1	B	90	HIS
1	B	111	HIS
1	B	129	ASN
1	B	164	ASN
1	B	182	ASN
1	B	191	HIS
1	B	211	HIS
1	B	247	HIS
1	B	337	ASN
1	B	362	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	370	GLN
1	B	388	GLN
1	B	459	HIS
1	B	481	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	DGB	B	1002	-	31,31,31	1.34	4 (12%)	39,39,39	1.47	10 (25%)
2	DGB	A	1001	-	31,31,31	1.04	4 (12%)	39,39,39	1.44	6 (15%)

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	DGB	B	1002	-	-	7/21/31/31	0/3/3/3
2	DGB	A	1001	-	-	5/21/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1002	DGB	CAC-CAX	-4.93	1.37	1.48
2	A	1001	DGB	CAC-CAX	-3.42	1.41	1.48
2	B	1002	DGB	CAZ-CAD	-3.28	1.38	1.47
2	B	1002	DGB	CAC-CAD	3.04	1.40	1.33
2	A	1001	DGB	CAZ-CAD	-2.30	1.40	1.47
2	A	1001	DGB	CAC-CAD	2.27	1.38	1.33
2	B	1002	DGB	CBA-CAY	2.17	1.53	1.50
2	A	1001	DGB	CBA-CAY	2.16	1.53	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	DGB	CAC-CAX-NAW	4.71	123.85	114.97
2	B	1002	DGB	CAZ-CAD-CAC	-3.48	118.95	126.91
2	A	1001	DGB	CAI-NAV-CAM	3.23	122.43	116.85
2	B	1002	DGB	CAS-CAU-NBC	-3.19	105.97	110.82
2	A	1001	DGB	CAP-NAW-CAX	3.17	127.19	122.54
2	B	1002	DGB	CAI-NAV-CAM	2.96	121.96	116.85
2	A	1001	DGB	OAA-CAX-CAC	-2.80	116.64	123.03
2	A	1001	DGB	CAU-NBC-CAT	2.55	117.53	112.62
2	B	1002	DGB	CAU-NBC-CAT	2.50	117.44	112.62
2	B	1002	DGB	OAA-CAX-CAC	-2.49	117.35	123.03
2	A	1001	DGB	CAD-CAC-CAX	2.45	126.34	121.56
2	B	1002	DGB	OAB-CAY-NBC	-2.28	118.57	122.34
2	B	1002	DGB	CAQ-CBB-CAR	-2.15	106.97	112.11
2	B	1002	DGB	CAC-CAX-NAW	2.06	118.85	114.97
2	B	1002	DGB	CBA-CAY-NBC	2.01	121.27	118.72
2	B	1002	DGB	CAN-CAO-CAQ	-2.00	106.53	113.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DGB	OAA-CAX-NAW-CAP
2	A	1001	DGB	CAC-CAX-NAW-CAP
2	B	1002	DGB	CAN-CAP-NAW-CAX

Continued on next page...

Continued from previous page...

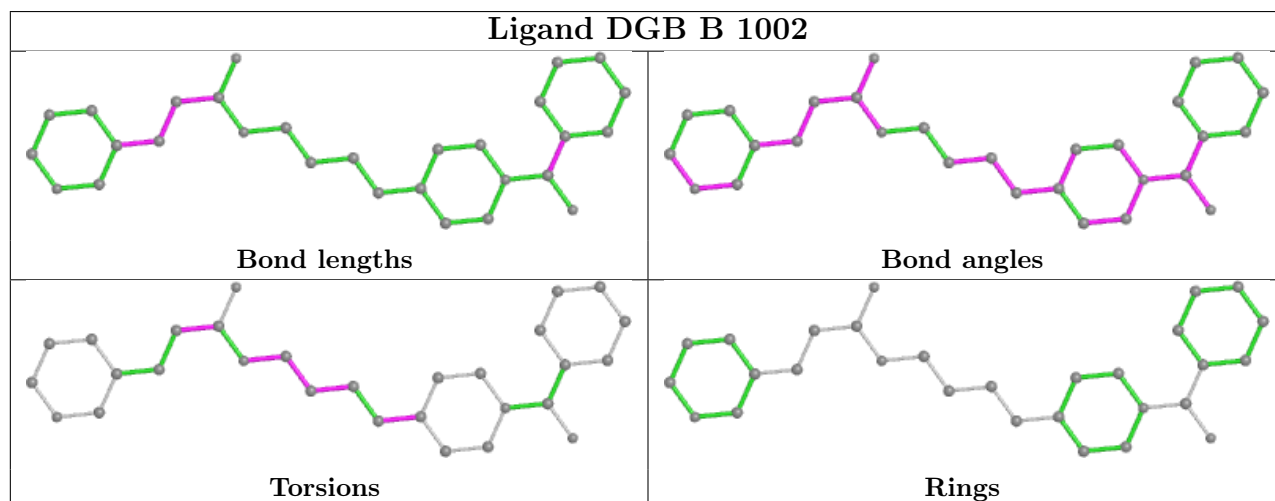
Mol	Chain	Res	Type	Atoms
2	B	1002	DGB	CAO-CAN-CAP-NAW
2	B	1002	DGB	CAO-CAQ-CBB-CAS
2	B	1002	DGB	CAD-CAC-CAX-OAA
2	A	1001	DGB	CAN-CAO-CAQ-CBB
2	B	1002	DGB	CAP-CAN-CAO-CAQ
2	B	1002	DGB	CAD-CAC-CAX-NAW
2	A	1001	DGB	CAD-CAC-CAX-OAA
2	A	1001	DGB	CAD-CAC-CAX-NAW
2	B	1002	DGB	CAO-CAQ-CBB-CAR

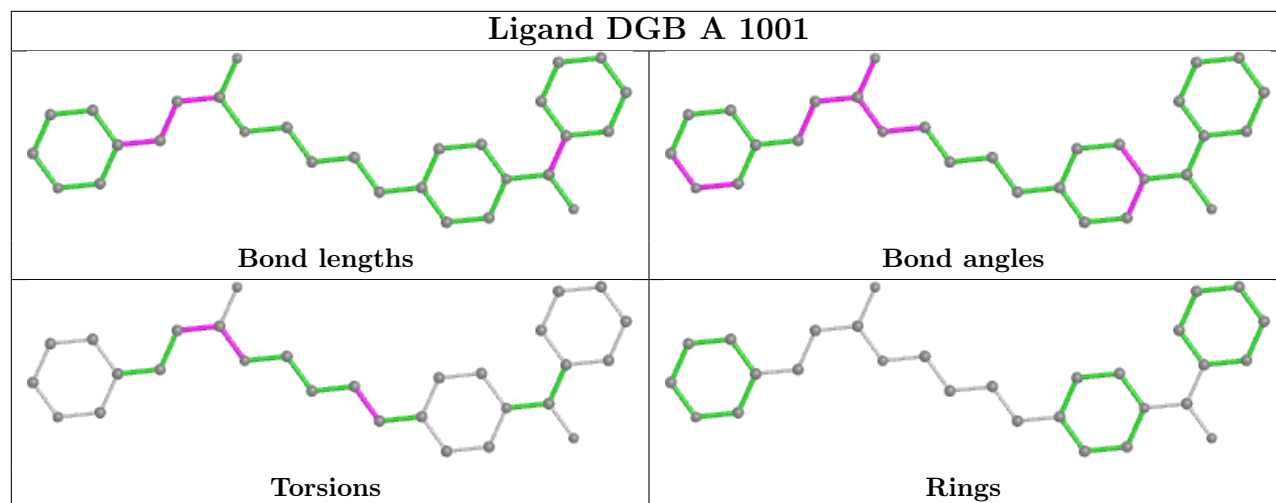
There are no ring outliers.

2 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	DGB	18	0
2	A	1001	DGB	14	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	463/491 (94%)	0.01	7 (1%) 73 73	4, 17, 34, 49	0
1	B	463/491 (94%)	-0.05	9 (1%) 66 65	5, 16, 34, 50	0
All	All	926/982 (94%)	-0.02	16 (1%) 70 69	4, 16, 34, 50	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	237	VAL	5.0
1	B	236	PRO	4.7
1	B	92	GLN	3.1
1	A	451	GLU	3.0
1	B	105	LEU	2.9
1	B	235	ASP	2.6
1	B	76	THR	2.5
1	A	298	LEU	2.5
1	B	103	TYR	2.4
1	B	240	TYR	2.2
1	A	233	THR	2.2
1	A	450	LEU	2.1
1	A	92	GLN	2.1
1	B	418	VAL	2.1
1	A	73	LYS	2.1
1	A	455	HIS	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](#)

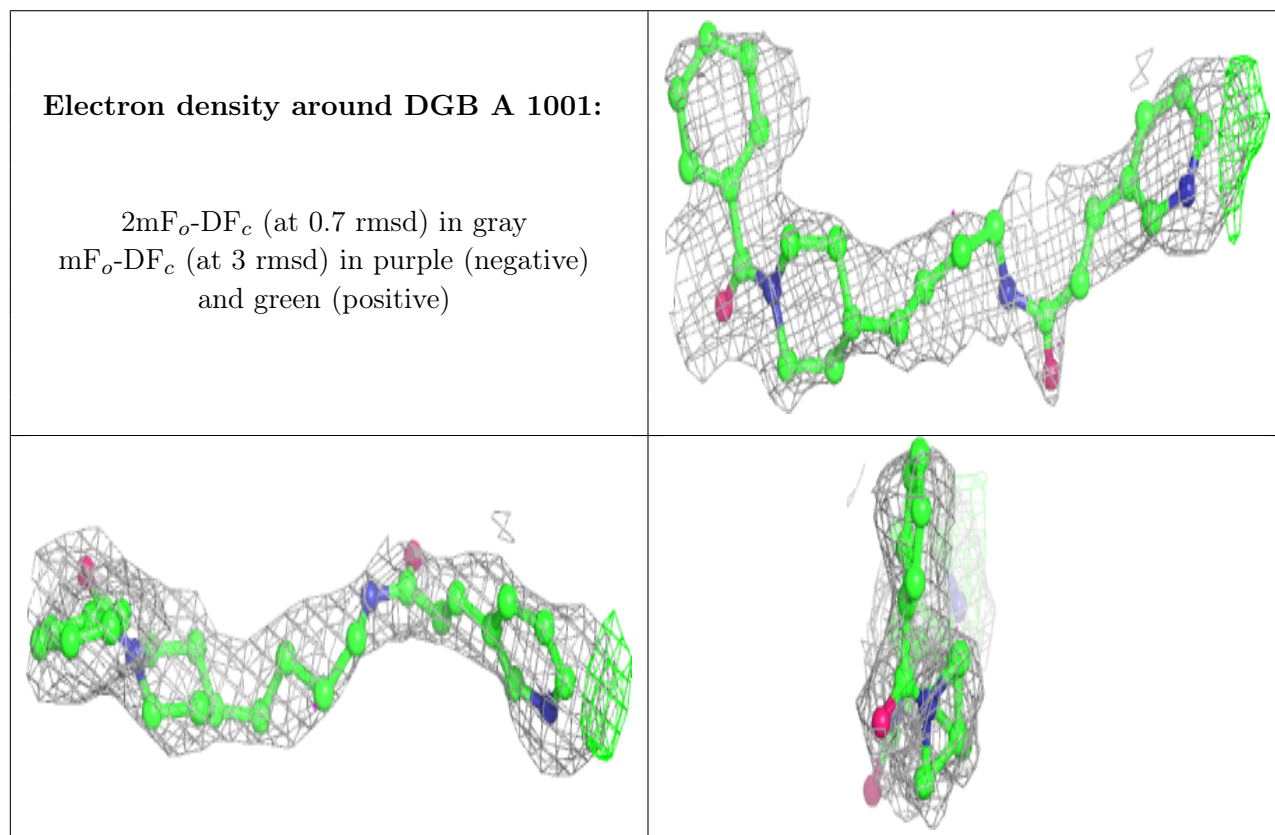
There are no monosaccharides in this entry.

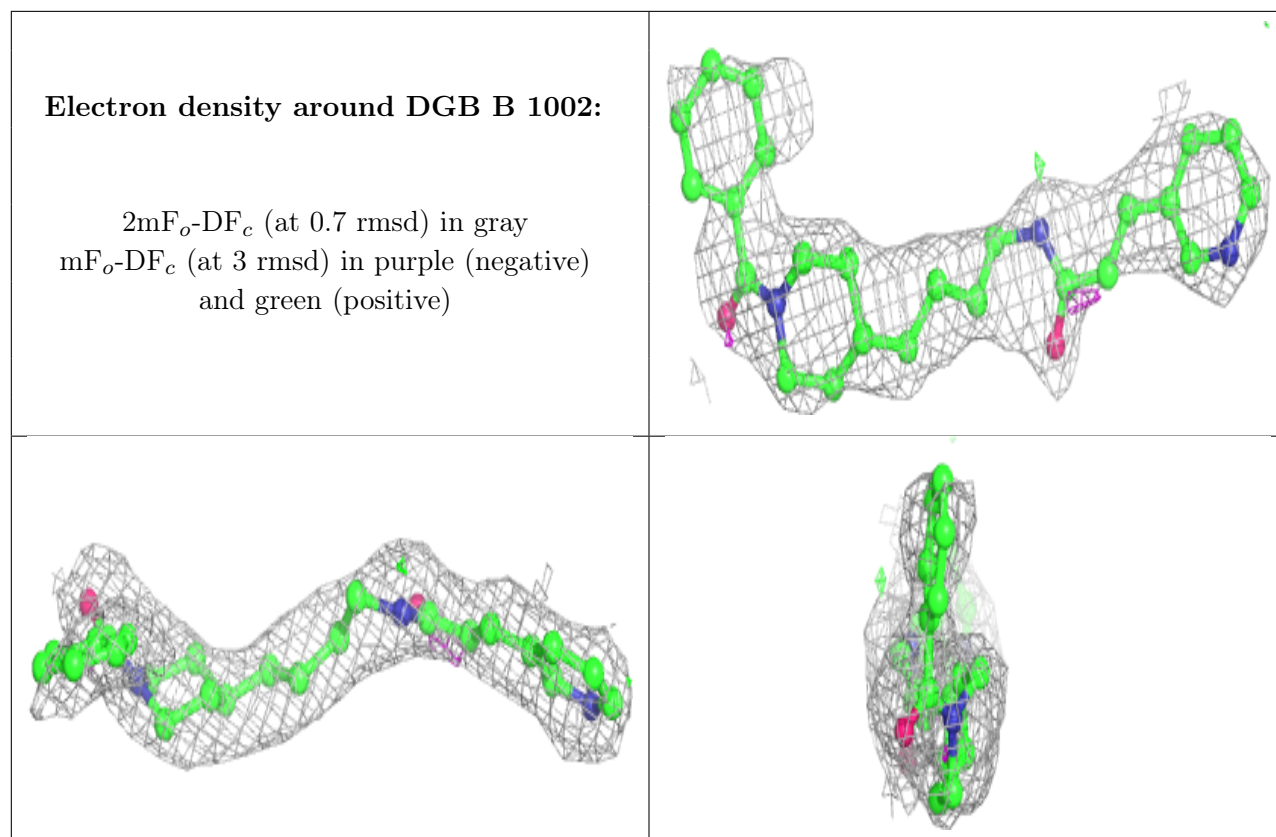
6.4 Ligands [i](#)

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	DGB	A	1001	29/29	0.85	0.27	18,22,28,29	0
2	DGB	B	1002	29/29	0.88	0.24	12,18,23,24	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.