



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:02 AM UTC

PDB ID : 1HE8 / pdb_00001he8
Title : Ras G12V - PI 3-kinase gamma complex
Authors : Pacold, M.E.; Suire, S.; Perisic, O.; Lara-Gonzalez, S.; Davis, C.T.; Hawkins, P.T.; Walker, E.H.; Stephens, L.; Eccleston, J.F.; Williams, R.L.
Deposited on : 2000-11-20
Resolution : 3.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

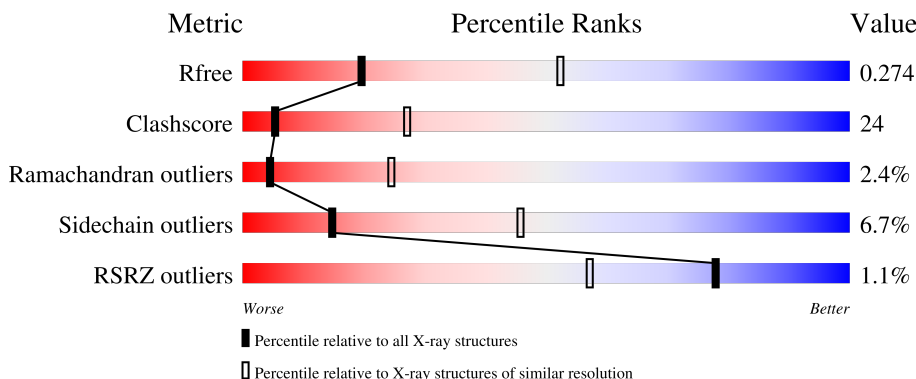
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	965	40% 32% 5% 22%
2	B	166	55% 39% 5%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7434 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 PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT, GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	0	0
			6069	3894	1033	1107	35			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	LYS	VAL	engineered mutation	UNP P48736
A	326	ALA	VAL	engineered mutation	UNP P48736

- Molecule 2 is a protein called TRANSFORMING PROTEIN P21/H-RAS-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1326	827	228	264	7			

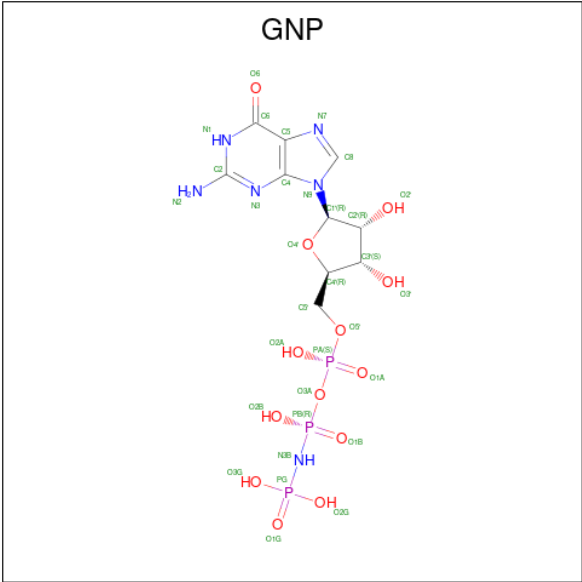
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	VAL	GLY	engineered mutation	UNP P01112

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

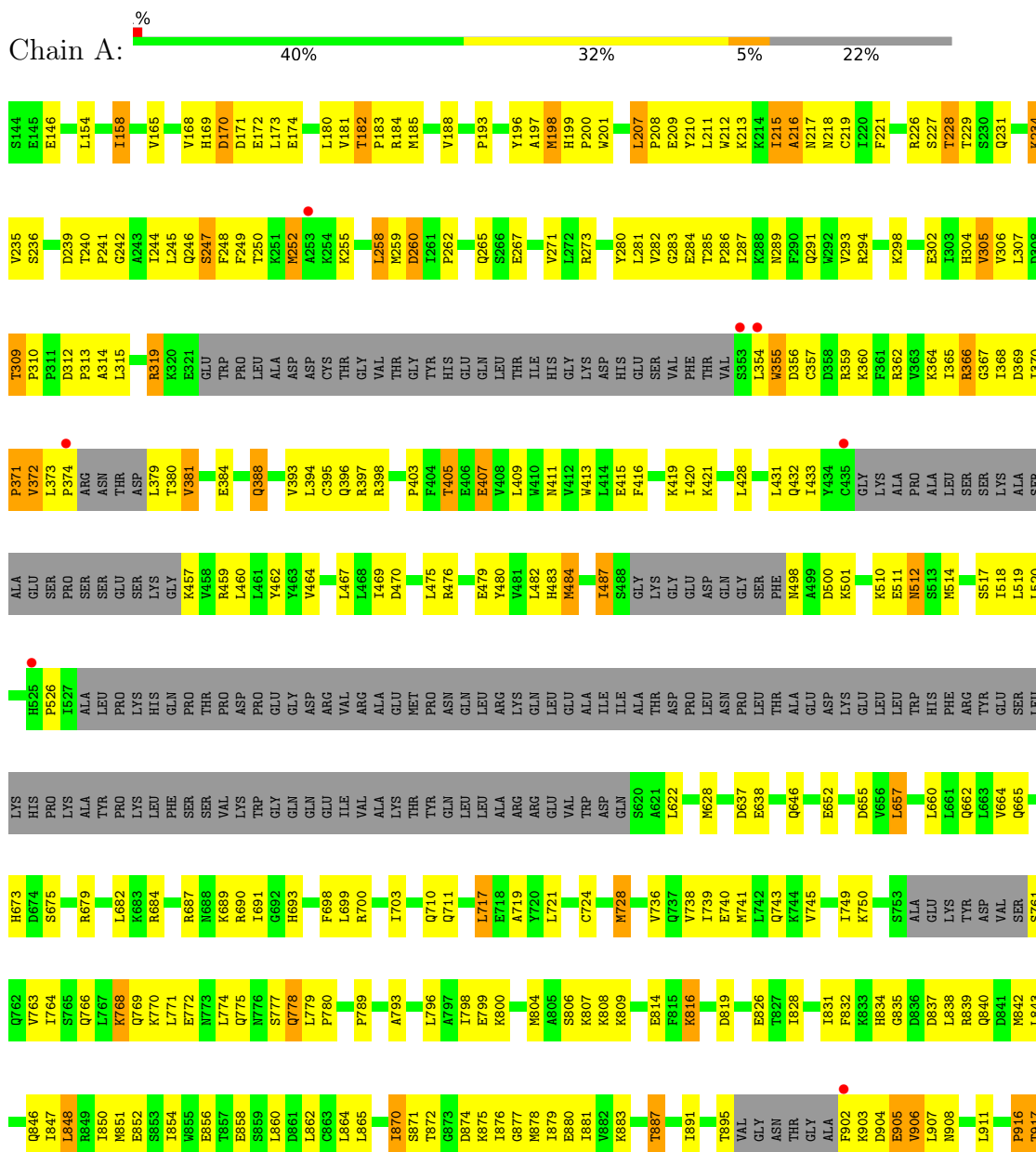
- Molecule 5 is water.

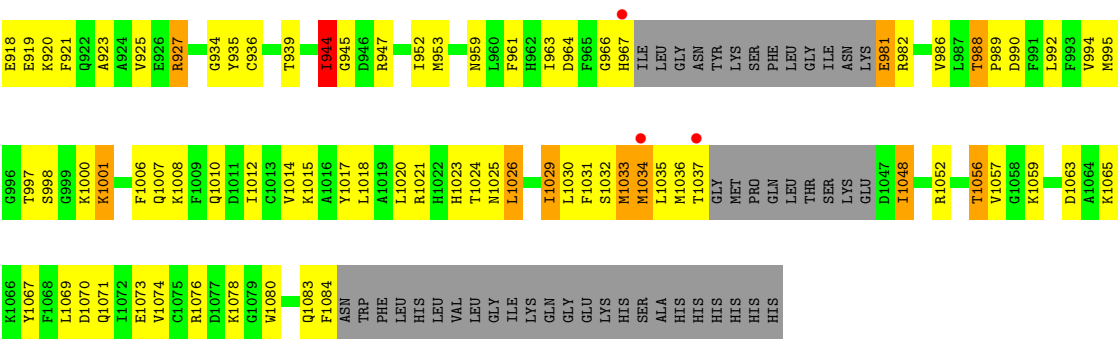
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	5	Total	O	0	0
			5	5		

3 Residue-property plots

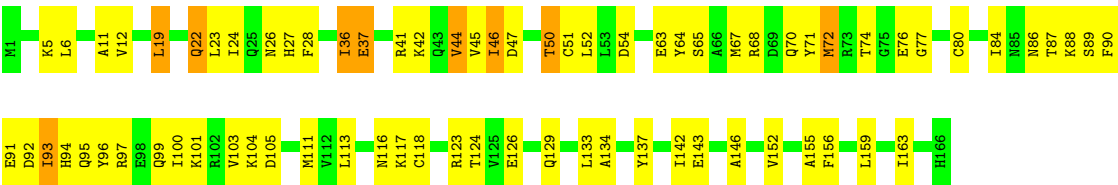
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUBUNIT, GAMMA ISO-FORM





● Molecule 2: TRANSFORMING PROTEIN P21/H-RAS-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.64Å 113.64Å 183.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	52.03 – 3.00 52.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (52.03-3.00) 91.6 (52.03-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.280 0.210 , 0.274	Depositor DCC
R_{free} test set	1510 reflections (5.86%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 108.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7434	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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

5.1 Standard geometry

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

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	0.55	0/6192	0.89	11/8364 (0.1%)
2	B	0.67	0/1345	1.02	3/1815 (0.2%)
All	All	0.57	0/7537	0.92	14/10179 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	ILE	N-CA-C	-9.27	102.86	111.67
1	A	309	THR	CA-C-N	6.34	124.29	119.66
1	A	309	THR	C-N-CA	6.34	124.29	119.66
1	A	484	MET	N-CA-C	6.29	118.14	110.41
2	B	152	VAL	N-CA-C	5.87	116.00	110.30
2	B	22	GLN	N-CA-C	-5.83	104.55	111.03
1	A	309	THR	N-CA-C	5.83	117.16	109.93
1	A	381	VAL	N-CA-C	5.34	116.36	108.45
1	A	199	HIS	CA-C-N	5.29	125.21	119.76
1	A	199	HIS	C-N-CA	5.29	125.21	119.76
1	A	691	ILE	N-CA-C	-5.14	105.69	110.53
1	A	158	ILE	CB-CA-C	-5.09	105.36	111.88
1	A	228	THR	N-CA-C	-5.07	107.38	113.21
1	A	388	GLN	N-CA-C	5.03	117.79	109.85

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	6069	0	6121	303	0
2	B	1326	0	1301	56	0
3	B	1	0	0	0	0
4	B	32	0	13	0	0
5	A	1	0	0	0	0
5	B	5	0	0	1	0
All	All	7434	0	7435	358	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 24.

All (358) 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:228:THR:HB	2:B:41:ARG:HB3	1.36	1.06
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.53	0.89
1:A:372:VAL:HG12	1:A:373:LEU:H	1.42	0.84
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.13	0.84
1:A:745:VAL:HG21	1:A:774:LEU:HD11	1.58	0.83
1:A:847:ILE:HG22	1:A:851:MET:HE3	1.61	0.82
1:A:255:LYS:HD3	1:A:258:LEU:HD12	1.64	0.80
2:B:133:LEU:HD11	2:B:137:TYR:CZ	2.17	0.78
2:B:19:LEU:HD12	2:B:146:ALA:HB2	1.66	0.77
1:A:895:THR:HG22	1:A:902:PHE:HB2	1.68	0.75
1:A:479:GLU:HG2	1:A:519:LEU:HD13	1.68	0.75
1:A:917:THR:HG23	1:A:920:LYS:HB2	1.68	0.74
1:A:750:LYS:HE3	1:A:809:LYS:HG2	1.70	0.73
1:A:992:LEU:HA	1:A:995:MET:HE3	1.71	0.73
1:A:366:ARG:HB2	1:A:517:SER:HB3	1.72	0.72
1:A:903:LYS:O	1:A:906:VAL:HG23	1.90	0.72
1:A:989:PRO:HG2	1:A:1080:TRP:NE1	2.05	0.72
1:A:741:MET:HE1	1:A:779:LEU:HA	1.73	0.71
1:A:420:ILE:HD12	1:A:475:LEU:CD2	2.21	0.70
1:A:736:VAL:O	1:A:740:GLU:HB2	1.91	0.70
1:A:420:ILE:HG23	1:A:475:LEU:HD22	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:LEU:HD12	1:A:994:VAL:HG21	1.74	0.69
1:A:761:SER:HB3	1:A:764:ILE:HG13	1.74	0.68
1:A:1048:ILE:O	1:A:1048:ILE:HD13	1.92	0.68
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.75	0.68
1:A:245:LEU:HD21	1:A:307:LEU:HD13	1.75	0.68
1:A:356:ASP:HB3	1:A:359:ARG:HG3	1.76	0.68
1:A:779:LEU:HD23	1:A:780:PRO:HD2	1.76	0.67
1:A:355:TRP:HB3	1:A:359:ARG:CZ	2.25	0.67
1:A:457:LYS:HD3	1:A:459:ARG:HH21	1.57	0.67
1:A:498:ASN:HD21	1:A:500:ASP:HB2	1.61	0.66
1:A:847:ILE:CG2	1:A:851:MET:HE3	2.24	0.66
1:A:364:LYS:HE2	1:A:366:ARG:NH2	2.12	0.65
1:A:184:ARG:O	1:A:188:VAL:HG23	1.97	0.65
1:A:860:LEU:HD21	1:A:1015:LYS:HD3	1.79	0.64
1:A:816:LYS:HB2	1:A:816:LYS:NZ	2.13	0.64
1:A:240:THR:HG22	1:A:242:GLY:N	2.12	0.64
1:A:518:ILE:HD12	1:A:520:LEU:CD1	2.28	0.64
1:A:921:PHE:O	1:A:925:VAL:HG23	1.98	0.64
1:A:796:LEU:HD22	1:A:798:ILE:HG13	1.80	0.63
1:A:947:ARG:NH2	1:A:963:ILE:O	2.30	0.63
2:B:97:ARG:HD3	2:B:101:LYS:HE2	1.80	0.63
1:A:518:ILE:HD12	1:A:520:LEU:HD11	1.78	0.63
1:A:761:SER:OG	1:A:763:VAL:HG12	1.98	0.63
2:B:68:ARG:O	2:B:72:MET:HB2	1.98	0.63
1:A:366:ARG:HE	1:A:366:ARG:HA	1.62	0.62
1:A:628:MET:HB3	1:A:1033:MET:HE1	1.82	0.62
2:B:45:VAL:HA	2:B:50:THR:HA	1.82	0.61
1:A:355:TRP:HB3	1:A:359:ARG:NH2	2.15	0.61
1:A:1006:PHE:O	1:A:1010:GLN:HG3	2.01	0.61
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.83	0.61
1:A:840:GLN:OE1	1:A:966:GLY:HA2	2.01	0.60
1:A:743:GLN:HA	1:A:832:PHE:HE2	1.67	0.60
1:A:887:THR:HG23	1:A:953:MET:HG2	1.83	0.60
1:A:168:VAL:HG12	1:A:170:ASP:H	1.67	0.60
2:B:92:ASP:HA	2:B:95:GLN:HG2	1.84	0.60
1:A:766:GLN:O	1:A:770:LYS:HG3	2.01	0.60
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.83	0.60
1:A:182:THR:OG1	1:A:183:PRO:HD3	2.02	0.60
1:A:743:GLN:HA	1:A:832:PHE:CE2	2.37	0.59
1:A:420:ILE:HD12	1:A:475:LEU:HD21	1.84	0.59
1:A:373:LEU:HG	1:A:374:PRO:HD2	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:LEU:HG	1:A:1034:MET:CG	2.31	0.59
1:A:169:HIS:CD2	1:A:476:ARG:HH12	2.21	0.59
1:A:379:LEU:HG	1:A:380:THR:H	1.66	0.59
2:B:64:TYR:O	2:B:67:MET:HG2	2.00	0.59
1:A:483:HIS:CD2	1:A:510:LYS:HA	2.36	0.59
2:B:113:LEU:HD23	2:B:134:ALA:HB2	1.83	0.59
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.84	0.59
1:A:397:ARG:HG2	1:A:416:PHE:CD2	2.37	0.58
1:A:771:LEU:HD12	1:A:798:ILE:HG23	1.85	0.58
1:A:287:ILE:O	1:A:293:VAL:HG21	2.03	0.58
1:A:370:ILE:HD12	1:A:514:MET:HE2	1.85	0.58
1:A:169:HIS:HD2	1:A:476:ARG:HH12	1.51	0.58
1:A:255:LYS:HG2	1:A:258:LEU:HB2	1.85	0.58
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.86	0.58
1:A:371:PRO:HG2	1:A:512:ASN:HA	1.86	0.57
1:A:622:LEU:HD11	1:A:854:ILE:HA	1.86	0.57
1:A:240:THR:HG22	1:A:242:GLY:H	1.67	0.57
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.86	0.57
1:A:476:ARG:HD2	1:A:480:TYR:OH	2.04	0.57
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.69	0.57
1:A:262:PRO:HB2	1:A:265:GLN:HB2	1.86	0.57
1:A:359:ARG:O	1:A:420:ILE:HG12	2.05	0.57
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.87	0.57
1:A:880:GLU:HG2	1:A:881:ILE:N	2.17	0.57
2:B:19:LEU:CD1	2:B:146:ALA:HB2	2.34	0.57
1:A:826:GLU:HG2	1:A:883:LYS:HZ3	1.69	0.56
1:A:367:GLY:HA3	1:A:409:LEU:HD23	1.87	0.56
1:A:657:LEU:HD11	1:A:690:ARG:HE	1.70	0.56
1:A:766:GLN:HA	1:A:769:GLN:OE1	2.05	0.56
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.35	0.55
1:A:936:CYS:O	1:A:939:THR:HG22	2.06	0.55
1:A:241:PRO:HD3	1:A:285:THR:O	2.06	0.55
1:A:236:SER:HB3	1:A:239:ASP:OD2	2.07	0.55
1:A:660:LEU:HD23	1:A:698:PHE:CE2	2.41	0.55
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.21	0.55
1:A:420:ILE:HD12	1:A:475:LEU:HD22	1.89	0.55
1:A:703:ILE:HD12	1:A:717:LEU:HD12	1.89	0.55
1:A:981:GLU:HG2	1:A:982:ARG:H	1.72	0.55
1:A:779:LEU:HD23	1:A:780:PRO:CD	2.37	0.54
1:A:146:GLU:HG2	1:A:319:ARG:HH21	1.73	0.54
1:A:842:MET:HE2	1:A:871:SER:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.89	0.54
1:A:798:ILE:HD12	1:A:798:ILE:H	1.72	0.54
1:A:804:MET:HE1	1:A:831:ILE:HD13	1.89	0.54
2:B:118:CYS:SG	2:B:143:GLU:HB3	2.47	0.54
1:A:200:PRO:HG3	1:A:282:VAL:CG2	2.37	0.54
1:A:231:GLN:OE1	1:A:252:MET:HE1	2.07	0.54
1:A:1065:LYS:O	1:A:1069:LEU:HG	2.08	0.54
2:B:123:ARG:HG2	2:B:124:THR:N	2.23	0.54
1:A:209:GLU:OE1	1:A:209:GLU:HA	2.07	0.53
1:A:739:ILE:HG22	1:A:878:MET:HE1	1.90	0.53
1:A:768:LYS:O	1:A:772:GLU:HG2	2.08	0.53
1:A:838:LEU:O	1:A:842:MET:HG3	2.09	0.53
1:A:816:LYS:HB2	1:A:816:LYS:HZ2	1.72	0.53
1:A:838:LEU:HD21	1:A:879:ILE:HD11	1.89	0.53
1:A:281:LEU:HD22	1:A:305:VAL:HG11	1.91	0.53
2:B:42:LYS:HG2	2:B:44:VAL:HG23	1.91	0.53
1:A:366:ARG:HH21	1:A:411:ASN:HB3	1.74	0.53
1:A:1073:GLU:HA	1:A:1076:ARG:HB2	1.91	0.53
2:B:72:MET:SD	2:B:99:GLN:HG2	2.49	0.53
1:A:652:GLU:HG2	1:A:655:ASP:OD2	2.09	0.52
1:A:662:GLN:CG	1:A:1033:MET:HE2	2.40	0.52
1:A:916:PRO:HD2	1:A:920:LYS:HG2	1.91	0.52
2:B:46:ILE:HG12	2:B:51:CYS:SG	2.50	0.52
1:A:312:ASP:HB3	1:A:315:LEU:HG	1.90	0.52
1:A:396:GLN:O	1:A:397:ARG:HD3	2.09	0.52
1:A:693:HIS:CG	1:A:789:PRO:HG3	2.44	0.52
1:A:874:ASP:OD1	1:A:875:LYS:HG3	2.10	0.52
2:B:126:GLU:HB2	2:B:129:GLN:HG3	1.91	0.52
1:A:750:LYS:NZ	1:A:808:LYS:HB3	2.25	0.52
2:B:28:PHE:HA	5:B:304:HOH:O	2.09	0.52
1:A:997:THR:HG22	1:A:998:SER:N	2.25	0.52
1:A:1025:ASN:O	1:A:1029:ILE:HG22	2.09	0.52
1:A:403:PRO:O	1:A:405:THR:HG23	2.10	0.52
1:A:917:THR:OG1	1:A:919:GLU:HG3	2.09	0.51
1:A:379:LEU:CG	1:A:380:THR:H	2.23	0.51
2:B:46:ILE:HG22	2:B:47:ASP:N	2.26	0.51
1:A:862:LEU:HD11	1:A:1012:ILE:HG22	1.92	0.51
2:B:87:THR:O	2:B:90:PHE:HB3	2.09	0.51
1:A:259:MET:O	1:A:260:ASP:HB3	2.09	0.51
1:A:920:LYS:O	1:A:923:ALA:HB3	2.11	0.51
1:A:852:GLU:CD	1:A:864:LEU:HB2	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASN:ND2	2:B:89:SER:HB3	2.26	0.51
1:A:870:ILE:HD13	1:A:871:SER:N	2.26	0.51
1:A:364:LYS:HD2	1:A:413:TRP:CZ2	2.47	0.50
2:B:116:ASN:O	2:B:117:LYS:HB2	2.11	0.50
1:A:739:ILE:HD13	1:A:872:THR:HB	1.91	0.50
1:A:768:LYS:HB2	1:A:768:LYS:HZ2	1.76	0.50
1:A:180:LEU:C	1:A:183:PRO:HD2	2.36	0.50
1:A:480:TYR:HB2	1:A:518:ILE:HG13	1.94	0.50
1:A:854:ILE:HG23	1:A:1023:HIS:HD2	1.77	0.50
1:A:227:SER:C	1:A:229:THR:H	2.20	0.50
1:A:246:GLN:O	1:A:250:THR:HG23	2.12	0.50
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.95	0.49
1:A:1034:MET:SD	1:A:1035:LEU:HD13	2.53	0.49
1:A:357:CYS:HB2	1:A:421:LYS:HB2	1.94	0.49
1:A:837:ASP:OD2	1:A:839:ARG:HB2	2.12	0.49
1:A:860:LEU:HD11	1:A:1015:LYS:HG2	1.94	0.49
1:A:903:LYS:C	1:A:905:GLU:H	2.19	0.49
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.93	0.49
1:A:154:LEU:O	1:A:158:ILE:HG12	2.12	0.49
1:A:221:PHE:CE1	1:A:234:LYS:HD2	2.46	0.49
1:A:854:ILE:HG23	1:A:1023:HIS:CD2	2.46	0.49
2:B:96:TYR:O	2:B:100:ILE:HG13	2.11	0.49
1:A:249:PHE:CD2	1:A:267:GLU:HB3	2.48	0.49
2:B:63:GLU:O	2:B:63:GLU:HG2	2.13	0.49
1:A:184:ARG:HD3	1:A:719:ALA:O	2.13	0.49
1:A:842:MET:HE2	1:A:871:SER:CB	2.43	0.49
1:A:240:THR:O	1:A:244:ILE:HG13	2.12	0.49
1:A:772:GLU:HA	1:A:775:GLN:HB3	1.94	0.48
1:A:793:ALA:HA	1:A:828:ILE:HD12	1.95	0.48
2:B:97:ARG:HG2	2:B:97:ARG:HH11	1.78	0.48
1:A:197:ALA:HA	1:A:689:LYS:NZ	2.29	0.48
2:B:142:ILE:HD12	2:B:155:ALA:HA	1.94	0.48
1:A:372:VAL:HG12	1:A:373:LEU:N	2.20	0.48
1:A:1007:GLN:HA	1:A:1010:GLN:HE21	1.78	0.48
1:A:741:MET:SD	1:A:779:LEU:HG	2.54	0.48
2:B:23:LEU:HD13	2:B:156:PHE:CG	2.49	0.48
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.48	0.48
1:A:988:THR:HG21	1:A:1083:GLN:HG3	1.95	0.48
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.14	0.48
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.95	0.48
1:A:1056:THR:HG22	1:A:1059:LYS:HD2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.96	0.48
1:A:273:ARG:NH2	1:A:819:ASP:OD2	2.45	0.47
1:A:662:GLN:HG3	1:A:1033:MET:HE2	1.95	0.47
1:A:838:LEU:HD22	1:A:877:GLY:HA3	1.96	0.47
1:A:215:ILE:HD12	1:A:215:ILE:O	2.14	0.47
1:A:262:PRO:HB2	1:A:265:GLN:CB	2.44	0.47
1:A:771:LEU:CD1	1:A:798:ILE:HG23	2.44	0.47
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.44	0.47
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.14	0.47
2:B:22:GLN:O	2:B:26:ASN:N	2.46	0.47
1:A:198:MET:HG3	1:A:280:TYR:CG	2.49	0.47
1:A:739:ILE:O	1:A:743:GLN:HB2	2.13	0.47
1:A:865:LEU:HD23	1:A:961:PHE:CD1	2.50	0.47
2:B:94:HIS:HD1	2:B:94:HIS:H	1.62	0.47
1:A:384:GLU:CD	1:A:396:GLN:HE21	2.22	0.47
1:A:908:ASN:HB2	1:A:994:VAL:HG22	1.96	0.47
1:A:384:GLU:HG3	1:A:398:ARG:HG2	1.95	0.47
1:A:1026:LEU:HD13	1:A:1030:LEU:HD12	1.96	0.47
1:A:235:VAL:HG11	1:A:244:ILE:HD13	1.96	0.47
1:A:738:VAL:O	1:A:741:MET:N	2.45	0.47
1:A:215:ILE:O	1:A:215:ILE:CG1	2.63	0.47
1:A:511:GLU:HB3	1:A:512:ASN:OD1	2.15	0.47
1:A:1034:MET:SD	1:A:1035:LEU:N	2.89	0.46
1:A:848:LEU:HG	1:A:864:LEU:HD13	1.96	0.46
2:B:104:LYS:O	2:B:105:ASP:C	2.57	0.46
1:A:865:LEU:HD23	1:A:961:PHE:CG	2.51	0.46
2:B:5:LYS:HA	2:B:54:ASP:HB2	1.98	0.46
2:B:97:ARG:HG3	2:B:137:TYR:CE2	2.50	0.46
1:A:196:TYR:O	1:A:689:LYS:HD2	2.16	0.46
1:A:215:ILE:O	1:A:215:ILE:HG13	2.16	0.46
1:A:240:THR:HG23	1:A:241:PRO:HD2	1.96	0.46
1:A:856:GLU:C	1:A:858:GLU:H	2.24	0.46
1:A:1014:VAL:O	1:A:1018:LEU:HG	2.16	0.46
2:B:5:LYS:O	2:B:76:GLU:HB2	2.16	0.46
1:A:945:GLY:O	1:A:986:VAL:HG23	2.16	0.46
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.16	0.46
1:A:354:LEU:N	1:A:354:LEU:HD22	2.31	0.46
1:A:927:ARG:HD3	1:A:959:ASN:HB2	1.98	0.46
1:A:397:ARG:HG2	1:A:416:PHE:CE2	2.51	0.46
1:A:660:LEU:O	1:A:664:VAL:HG23	2.16	0.46
1:A:944:ILE:HG22	1:A:967:HIS:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:HG3	1:A:282:VAL:HG23	1.97	0.46
1:A:750:LYS:HG3	1:A:809:LYS:CG	2.46	0.46
1:A:699:LEU:O	1:A:703:ILE:HG13	2.16	0.45
2:B:52:LEU:C	2:B:52:LEU:HD13	2.41	0.45
1:A:209:GLU:O	1:A:213:LYS:HG3	2.15	0.45
1:A:848:LEU:HD12	1:A:848:LEU:HA	1.81	0.45
1:A:368:ILE:CG2	1:A:433:ILE:HD11	2.47	0.45
1:A:637:ASP:O	1:A:638:GLU:C	2.59	0.45
1:A:172:GLU:HG2	1:A:673:HIS:CD2	2.52	0.45
1:A:1001:LYS:NZ	1:A:1001:LYS:HB2	2.31	0.45
1:A:768:LYS:HB2	1:A:768:LYS:NZ	2.31	0.45
1:A:770:LYS:O	1:A:774:LEU:HG	2.16	0.45
2:B:23:LEU:C	2:B:23:LEU:HD23	2.41	0.45
2:B:36:ILE:O	2:B:37:GLU:HB2	2.17	0.45
1:A:221:PHE:HE1	1:A:234:LYS:HD2	1.81	0.45
1:A:364:LYS:O	1:A:518:ILE:HA	2.17	0.45
1:A:388:GLN:HG2	1:A:393:VAL:HA	1.99	0.45
2:B:91:GLU:O	2:B:94:HIS:ND1	2.50	0.45
1:A:255:LYS:CD	1:A:258:LEU:HD12	2.43	0.45
1:A:879:ILE:HD12	1:A:879:ILE:N	2.32	0.45
1:A:838:LEU:HD21	1:A:879:ILE:CD1	2.47	0.44
1:A:242:GLY:O	1:A:246:GLN:HG3	2.17	0.44
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.98	0.44
1:A:806:SER:O	1:A:807:LYS:C	2.59	0.44
1:A:832:PHE:CE2	1:A:876:ILE:HD11	2.52	0.44
1:A:990:ASP:O	1:A:994:VAL:HG23	2.17	0.44
1:A:703:ILE:CD1	1:A:717:LEU:HD12	2.48	0.44
1:A:745:VAL:O	1:A:749:ILE:HG22	2.17	0.44
1:A:1029:ILE:C	1:A:1029:ILE:HD13	2.42	0.44
2:B:87:THR:O	2:B:88:LYS:C	2.59	0.44
1:A:367:GLY:HA3	1:A:409:LEU:CD2	2.47	0.44
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.18	0.44
1:A:431:LEU:HD11	1:A:518:ILE:HG21	2.00	0.44
1:A:460:LEU:HG	1:A:487:ILE:HD11	1.99	0.44
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.53	0.44
2:B:22:GLN:O	2:B:26:ASN:HA	2.18	0.44
2:B:100:ILE:HG21	2:B:111:MET:HE2	1.98	0.44
1:A:470:ASP:OD1	1:A:470:ASP:C	2.61	0.44
1:A:843:LEU:CG	1:A:1034:MET:HG3	2.36	0.44
1:A:903:LYS:C	1:A:905:GLU:N	2.76	0.44
2:B:41:ARG:HG3	2:B:52:LEU:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:O	1:A:172:GLU:C	2.61	0.44
1:A:364:LYS:HD2	1:A:413:TRP:CE2	2.52	0.44
1:A:1032:SER:C	1:A:1036:MET:HE3	2.43	0.44
2:B:77:GLY:HA3	2:B:163:ILE:HD11	1.99	0.44
2:B:84:ILE:HG13	2:B:116:ASN:O	2.17	0.44
1:A:252:MET:HE2	1:A:259:MET:HG2	2.00	0.43
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.53	0.43
1:A:283:GLY:O	1:A:285:THR:N	2.51	0.43
1:A:309:THR:HA	1:A:310:PRO:HD3	1.85	0.43
1:A:469:ILE:N	1:A:469:ILE:HD12	2.33	0.43
1:A:1008:LYS:O	1:A:1012:ILE:HG13	2.18	0.43
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.53	0.43
1:A:217:ASN:C	1:A:219:CYS:H	2.26	0.43
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.99	0.43
1:A:684:ARG:HD3	1:A:687:ARG:HH21	1.84	0.43
1:A:982:ARG:HH11	1:A:982:ARG:HG3	1.82	0.43
2:B:41:ARG:CD	2:B:52:LEU:HD11	2.49	0.43
2:B:101:LYS:O	2:B:105:ASP:N	2.51	0.43
1:A:428:LEU:HD23	1:A:467:LEU:HA	2.01	0.43
1:A:741:MET:CG	1:A:774:LEU:HD22	2.49	0.43
1:A:1025:ASN:C	1:A:1025:ASN:HD22	2.25	0.43
1:A:903:LYS:O	1:A:905:GLU:N	2.52	0.43
2:B:71:TYR:CD1	2:B:72:MET:N	2.87	0.43
2:B:71:TYR:CE1	2:B:72:MET:HE3	2.54	0.43
1:A:208:PRO:HB3	1:A:210:TYR:CE2	2.55	0.42
1:A:464:VAL:HG12	1:A:484:MET:HE3	2.00	0.42
1:A:1059:LYS:HD3	1:A:1063:ASP:OD1	2.18	0.42
2:B:80:CYS:HB3	2:B:93:ILE:HD11	2.01	0.42
1:A:850:ILE:O	1:A:854:ILE:HG13	2.19	0.42
1:A:870:ILE:HD13	1:A:871:SER:H	1.84	0.42
1:A:911:LEU:HD23	1:A:911:LEU:HA	1.82	0.42
1:A:1056:THR:HG23	1:A:1067:TYR:CD2	2.55	0.42
2:B:99:GLN:O	2:B:103:VAL:HG23	2.20	0.42
1:A:271:VAL:HG23	1:A:282:VAL:HG12	2.01	0.42
1:A:741:MET:HE1	1:A:778:GLN:O	2.19	0.42
1:A:1074:VAL:O	1:A:1078:LYS:HG2	2.19	0.42
1:A:306:VAL:O	1:A:306:VAL:HG13	2.19	0.42
1:A:428:LEU:HD23	1:A:428:LEU:HA	1.79	0.42
1:A:480:TYR:HB2	1:A:518:ILE:CG1	2.48	0.42
1:A:1080:TRP:CE3	1:A:1084:PHE:HE1	2.37	0.42
2:B:84:ILE:HD11	2:B:117:LYS:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:LEU:HD11	2:B:137:TYR:OH	2.20	0.42
1:A:196:TYR:CE2	1:A:689:LYS:HE3	2.54	0.42
1:A:989:PRO:HB2	1:A:1080:TRP:CZ2	2.55	0.42
1:A:259:MET:O	1:A:260:ASP:CB	2.67	0.42
1:A:381:VAL:CG1	1:A:433:ILE:HG23	2.49	0.42
1:A:799:GLU:H	1:A:799:GLU:CD	2.26	0.42
1:A:215:ILE:HD12	1:A:216:ALA:O	2.19	0.42
1:A:365:ILE:HD13	1:A:518:ILE:HG22	2.02	0.42
1:A:675:SER:O	1:A:679:ARG:HG3	2.20	0.42
1:A:800:LYS:CB	1:A:814:GLU:HG3	2.50	0.42
1:A:997:THR:HG22	1:A:998:SER:H	1.83	0.42
1:A:286:PRO:HD2	1:A:289:ASN:HD22	1.85	0.42
1:A:851:MET:HG2	1:A:1020:LEU:HD21	2.02	0.42
1:A:464:VAL:HG21	1:A:482:LEU:HB3	2.02	0.42
1:A:158:ILE:HD11	1:A:721:LEU:HD12	2.02	0.41
1:A:226:ARG:HG2	1:A:259:MET:O	2.20	0.41
1:A:395:CYS:SG	1:A:416:PHE:HB3	2.60	0.41
1:A:779:LEU:HD23	1:A:780:PRO:N	2.35	0.41
1:A:826:GLU:OE1	1:A:883:LYS:HD3	2.20	0.41
1:A:952:ILE:HD11	1:A:986:VAL:HG21	2.02	0.41
1:A:215:ILE:HD12	1:A:215:ILE:C	2.45	0.41
1:A:464:VAL:HB	1:A:484:MET:HA	2.03	0.41
1:A:750:LYS:HZ1	1:A:808:LYS:HB3	1.86	0.41
1:A:1024:THR:HG21	1:A:1057:VAL:HG22	2.02	0.41
2:B:88:LYS:O	2:B:91:GLU:N	2.53	0.41
1:A:207:LEU:HA	1:A:294:ARG:NH1	2.35	0.41
1:A:360:LYS:HA	1:A:419:LYS:HA	2.02	0.41
1:A:362:ARG:HB3	1:A:415:GLU:HG3	2.03	0.41
1:A:862:LEU:N	1:A:862:LEU:HD22	2.36	0.41
2:B:24:ILE:HD13	2:B:24:ILE:HA	1.89	0.41
1:A:700:ARG:HH11	1:A:700:ARG:HG2	1.86	0.41
2:B:92:ASP:HA	2:B:95:GLN:CG	2.51	0.41
1:A:247:SER:O	1:A:248:PHE:C	2.64	0.41
1:A:834:HIS:ND1	1:A:835:GLY:N	2.69	0.41
1:A:1026:LEU:HA	1:A:1029:ILE:CG2	2.50	0.41
2:B:93:ILE:HD12	2:B:93:ILE:HA	1.87	0.41
2:B:123:ARG:CG	2:B:124:THR:N	2.84	0.41
1:A:312:ASP:OD1	1:A:314:ALA:HB3	2.21	0.41
1:A:369:ASP:CG	1:A:407:GLU:HG3	2.46	0.41
1:A:394:LEU:HB2	1:A:395:CYS:H	1.74	0.41
1:A:665:GLN:HB3	1:A:1037:THR:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:GLN:HG3	1:A:711:GLN:N	2.35	0.40
2:B:6:LEU:HG	2:B:159:LEU:HD23	2.02	0.40
1:A:356:ASP:HB3	1:A:359:ARG:CG	2.47	0.40
1:A:433:ILE:HB	1:A:462:TYR:HB2	2.04	0.40
1:A:887:THR:CG2	1:A:953:MET:HG2	2.49	0.40
1:A:738:VAL:O	1:A:739:ILE:C	2.63	0.40
1:A:854:ILE:HG21	1:A:1020:LEU:HD23	2.02	0.40
1:A:419:LYS:O	1:A:420:ILE:C	2.64	0.40
1:A:476:ARG:HD3	1:A:476:ARG:HA	1.88	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	729/965 (76%)	625 (86%)	87 (12%)	17 (2%)	5	25
2	B	164/166 (99%)	141 (86%)	19 (12%)	4 (2%)	4	24
All	All	893/1131 (79%)	766 (86%)	106 (12%)	21 (2%)	4	24

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ALA
2	B	46	ILE
1	A	260	ASP
1	A	778	GLN
1	A	906	VAL
1	A	916	PRO
1	A	170	ASP
1	A	284	GLU
1	A	405	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	904	ASP
1	A	964	ASP
2	B	37	GLU
1	A	218	ASN
1	A	371	PRO
1	A	777	SER
2	B	11	ALA
2	B	50	THR
1	A	247	SER
1	A	298	LYS
1	A	944	ILE
1	A	526	PRO

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	679/862 (79%)	633 (93%)	46 (7%)	14	45
2	B	145/145 (100%)	136 (94%)	9 (6%)	16	49
All	All	824/1007 (82%)	769 (93%)	55 (7%)	15	46

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	VAL
1	A	174	GLU
1	A	182	THR
1	A	198	MET
1	A	207	LEU
1	A	212	TRP
1	A	215	ILE
1	A	234	LYS
1	A	252	MET
1	A	258	LEU
1	A	305	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	319	ARG
1	A	355	TRP
1	A	366	ARG
1	A	372	VAL
1	A	407	GLU
1	A	487	ILE
1	A	501	LYS
1	A	512	ASN
1	A	646	GLN
1	A	657	LEU
1	A	682	LEU
1	A	717	LEU
1	A	728	MET
1	A	768	LYS
1	A	816	LYS
1	A	846	GLN
1	A	848	LEU
1	A	870	ILE
1	A	887	THR
1	A	905	GLU
1	A	917	THR
1	A	918	GLU
1	A	927	ARG
1	A	944	ILE
1	A	981	GLU
1	A	988	THR
1	A	1000	LYS
1	A	1001	LYS
1	A	1026	LEU
1	A	1029	ILE
1	A	1031	PHE
1	A	1033	MET
1	A	1034	MET
1	A	1048	ILE
1	A	1056	THR
2	B	12	VAL
2	B	19	LEU
2	B	27	HIS
2	B	44	VAL
2	B	65	SER
2	B	70	GLN
2	B	72	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	74	THR
2	B	93	ILE

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	148	GLN
1	A	153	GLN
1	A	295	HIS
1	A	299	ASN
1	A	304	HIS
1	A	388	GLN
1	A	389	HIS
1	A	392	GLN
1	A	396	GLN
1	A	432	GLN
1	A	471	HIS
1	A	483	HIS
1	A	498	ASN
1	A	629	GLN
1	A	646	GLN
1	A	710	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	846	GLN
1	A	892	GLN
1	A	908	ASN
1	A	922	GLN
1	A	951	ASN
1	A	1010	GLN
1	A	1023	HIS
1	A	1025	ASN
2	B	61	GLN
2	B	86	ASN
2	B	129	GLN

5.3.3 RNA ⓘ

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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GNP	B	202	3	34,34,34	2.32	5 (14%)	47,54,54	1.25	5 (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
4	GNP	B	202	3	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	202	GNP	PG-O1G	8.69	1.59	1.46
4	B	202	GNP	PA-O3A	6.18	1.66	1.59
4	B	202	GNP	PG-O3G	-4.72	1.44	1.56
4	B	202	GNP	PB-O2B	-3.84	1.46	1.56
4	B	202	GNP	PG-O2G	-3.43	1.47	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	202	GNP	O3G-PG-O1G	-4.85	101.30	113.45
4	B	202	GNP	O1B-PB-N3B	2.67	115.70	111.77
4	B	202	GNP	O1G-PG-N3B	-2.61	107.93	111.77
4	B	202	GNP	O2G-PG-O1G	-2.47	107.25	113.45
4	B	202	GNP	O2G-PG-O3G	2.00	112.97	107.59

There are no chirality outliers.

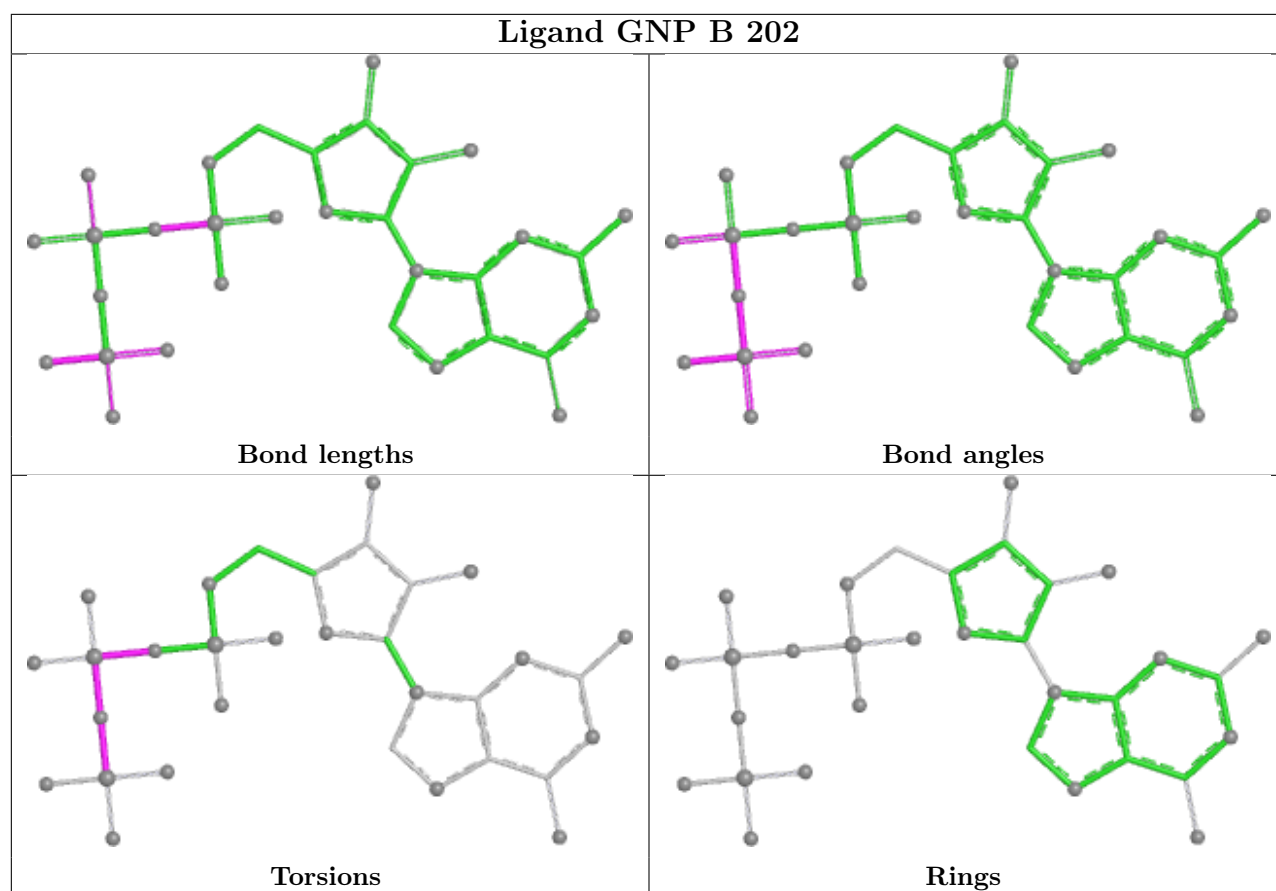
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	202	GNP	PB-N3B-PG-O1G
4	B	202	GNP	PG-N3B-PB-O1B
4	B	202	GNP	PG-N3B-PB-O3A
4	B	202	GNP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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	749/965 (77%)	-0.20	10 (1%) 75 53	23, 68, 122, 170	0
2	B	166/166 (100%)	-0.48	0 100 100	23, 51, 102, 132	0
All	All	915/1131 (80%)	-0.25	10 (1%) 78 57	23, 66, 119, 170	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1037	THR	2.9
1	A	967	HIS	2.7
1	A	374	PRO	2.6
1	A	353	SER	2.3
1	A	253	ALA	2.1
1	A	902	PHE	2.1
1	A	525	HIS	2.1
1	A	435	CYS	2.1
1	A	1034	MET	2.0
1	A	354	LEU	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](#)

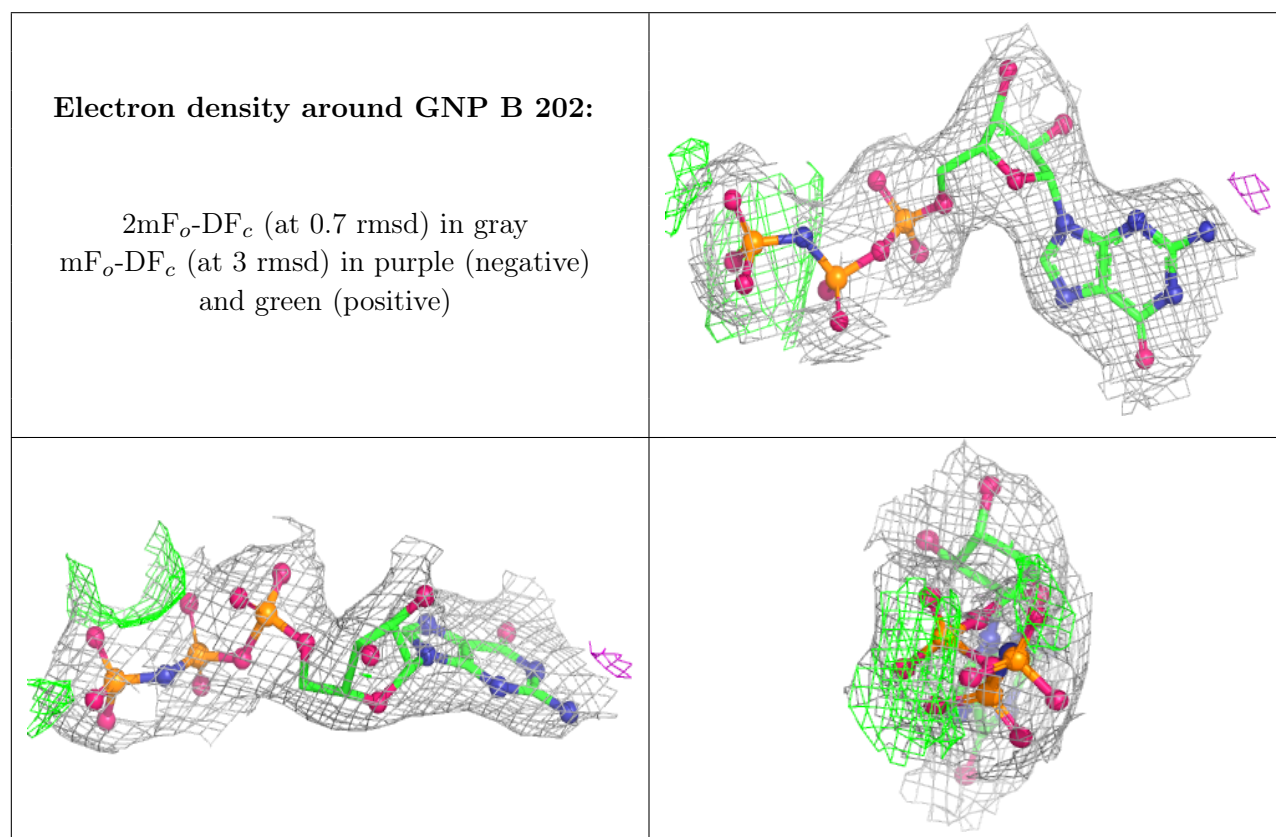
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	201	1/1	0.66	0.33	67,67,67,67	0
4	GNP	B	202	32/32	0.97	0.07	39,42,47,52	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.