



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:21 PM UTC

PDB ID : 3DPD / pdb_00003dpd
Title : Achieving multi-isoform PI3K inhibition in a series of substituted 3,4-Dihydro-2H-benzo[1,4]oxazines
Authors : Ceska, T.A.
Deposited on : 2008-07-08
Resolution : 2.85 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

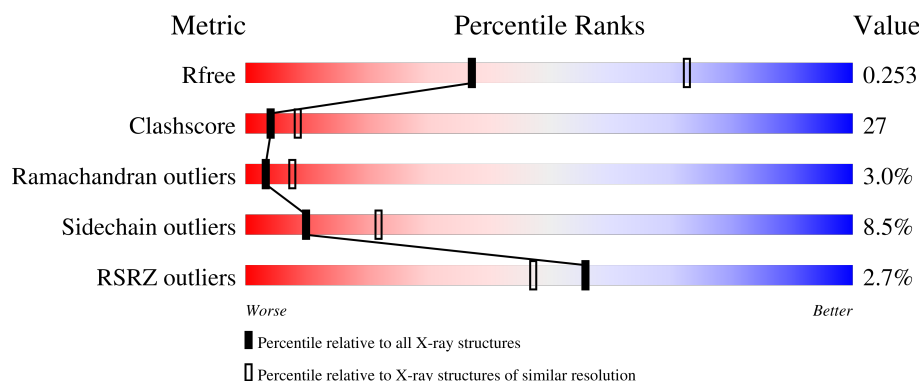
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	966	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6879 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.

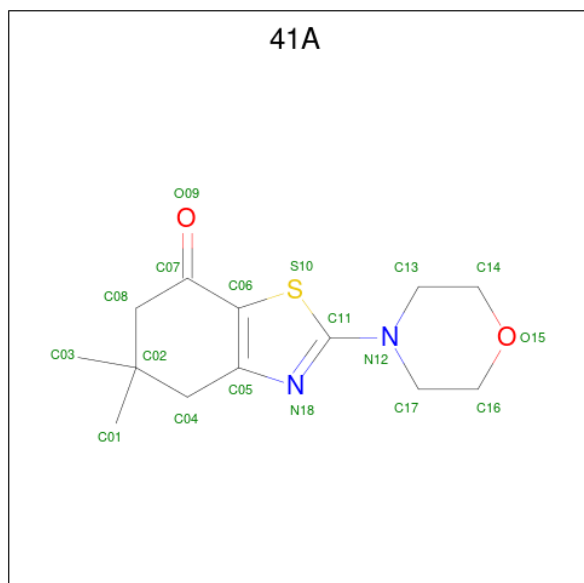
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	846	Total	C	N	O	S	0	0	0
			6861	4412	1168	1245	36			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	initiating methionine	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 5,5-dimethyl-2-morpholin-4-yl-5,6-dihydro-1,3-benzothiazol-7(4H)-one (CCD ID: 41A) (formula: C₁₃H₁₈N₂O₂S).

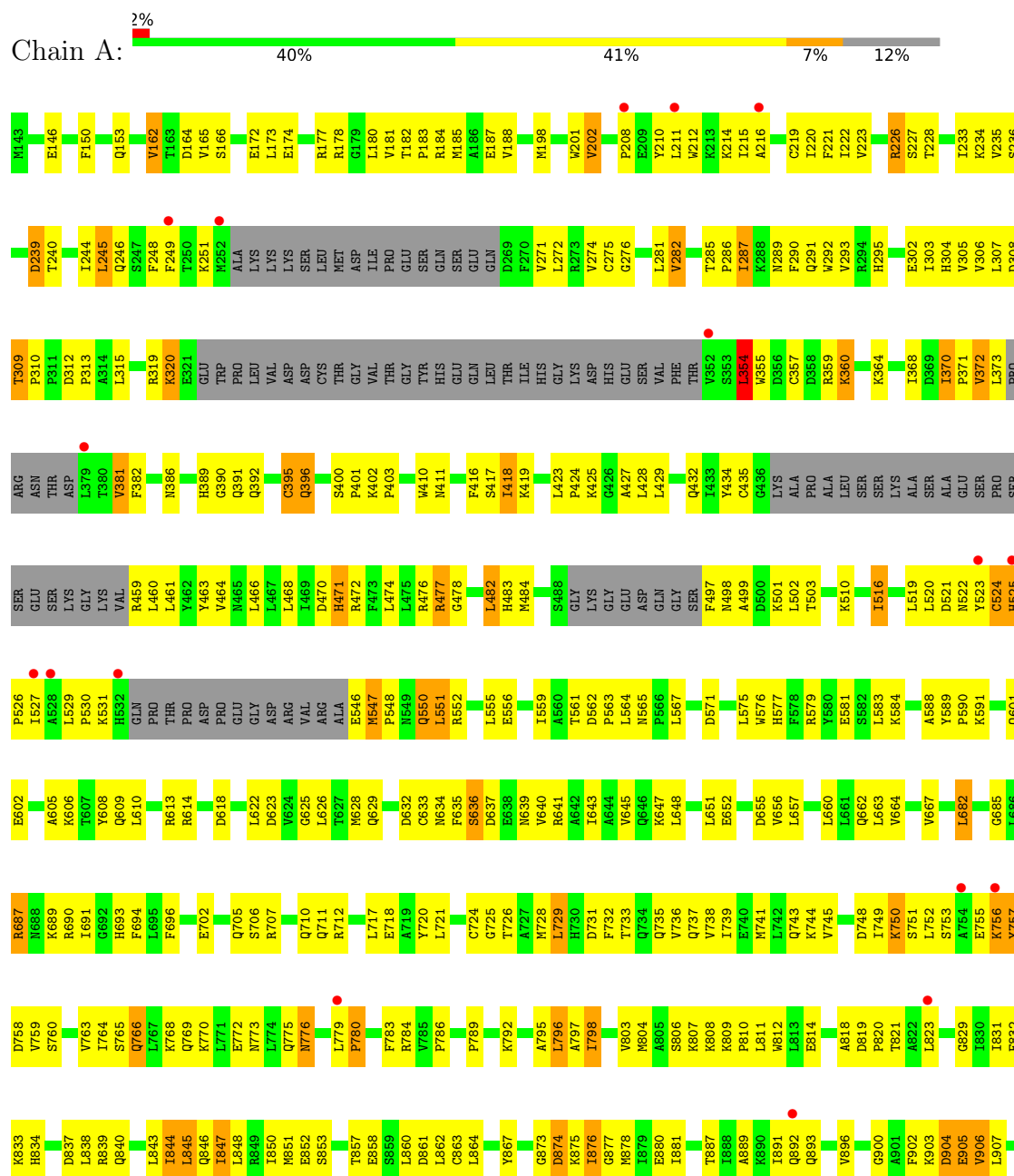


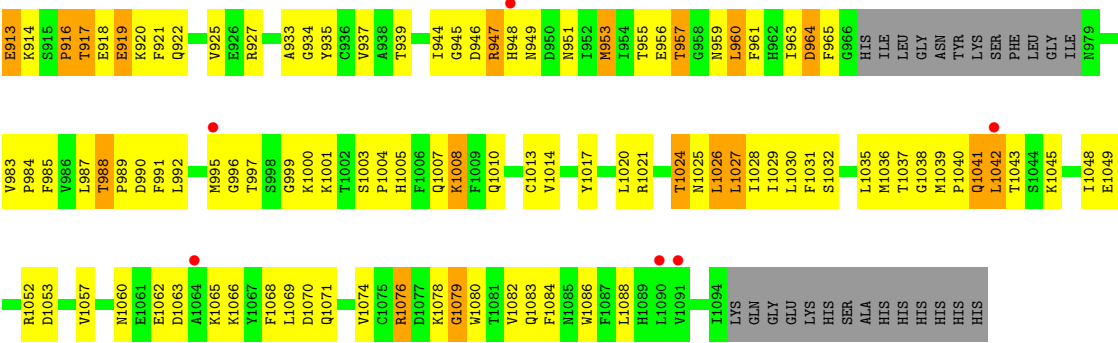
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	13	2	2	1		

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-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.23Å 67.77Å 105.87Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.85) 96.7 (30.00-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.85Å)	Xtriage
Refinement program	CNS, CNX 2002	Depositor
R, R_{free}	0.242 , 0.318 0.245 , 0.253	Depositor DCC
R_{free} test set	1175 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: 41A

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	0.48	0/7010	0.88	10/9483 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	988	THR	CA-C-N	6.28	126.76	119.47
1	A	988	THR	C-N-CA	6.28	126.76	119.47
1	A	228	THR	N-CA-C	-5.92	107.30	114.75
1	A	1008	LYS	N-CA-C	-5.83	104.84	111.14
1	A	503	THR	N-CA-C	5.38	118.03	110.23
1	A	1007	GLN	N-CA-C	-5.27	105.58	112.23
1	A	381	VAL	N-CA-C	5.22	115.42	108.27
1	A	844	ILE	CB-CA-C	-5.06	105.41	112.04
1	A	547	MET	CA-C-N	5.03	125.31	119.93
1	A	547	MET	C-N-CA	5.03	125.31	119.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6861	0	6909	379	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	18	0	18	0	0
All	All	6879	0	6927	379	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 27.

All (379) 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:629:GLN:HG2	1:A:1029:ILE:HG13	1.46	0.98
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.43	0.97
1:A:497:PHE:HB2	1:A:1042:LEU:HD22	1.45	0.96
1:A:1039:MET:HB3	1:A:1041:GLN:HE22	1.26	0.95
1:A:987:LEU:HD11	1:A:995:MET:HE1	1.50	0.93
1:A:418:ILE:HG12	1:A:419:LYS:H	1.34	0.93
1:A:1045:LYS:H	1:A:1045:LYS:HD2	1.35	0.90
1:A:221:PHE:HE1	1:A:234:LYS:HG2	1.36	0.90
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.54	0.88
1:A:689:LYS:HD2	1:A:728:MET:SD	2.17	0.83
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	1.93	0.83
1:A:798:ILE:HD12	1:A:798:ILE:H	1.44	0.81
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.13	0.79
1:A:497:PHE:HD1	1:A:1042:LEU:HB3	1.47	0.79
1:A:477:ARG:NE	1:A:522:ASN:HA	1.98	0.78
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.18	0.77
1:A:477:ARG:HE	1:A:522:ASN:HA	1.48	0.76
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.68	0.75
1:A:949:ASN:HB2	1:A:1083:GLN:HE22	1.48	0.74
1:A:222:ILE:HG22	1:A:303:ILE:HB	1.69	0.73
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.51	0.73
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.70	0.73
1:A:482:LEU:HD12	1:A:482:LEU:H	1.55	0.72
1:A:547:MET:HE2	1:A:552:ARG:HA	1.71	0.72
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.04	0.72
1:A:921:PHE:O	1:A:925:VAL:HG23	1.90	0.72
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.56	0.71
1:A:948:HIS:ND1	1:A:1086:TRP:HB3	2.07	0.70
1:A:202:VAL:HG12	1:A:290:PHE:HA	1.72	0.70
1:A:951:ASN:HA	1:A:963:ILE:HD11	1.73	0.70
1:A:531:LYS:HD2	1:A:608:TYR:HD1	1.57	0.70
1:A:579:ARG:HG2	1:A:610:LEU:HD11	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:O	1:A:177:ARG:HG3	1.92	0.69
1:A:499:ALA:HA	1:A:502:LEU:HD12	1.74	0.69
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.07	0.68
1:A:1076:ARG:HH11	1:A:1076:ARG:HB3	1.57	0.68
1:A:772:GLU:HG2	1:A:798:ILE:HG12	1.75	0.68
1:A:198:MET:SD	1:A:282:VAL:HG21	2.34	0.68
1:A:818:ALA:O	1:A:820:PRO:HD3	1.94	0.68
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.76	0.68
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.75	0.68
1:A:274:VAL:HA	1:A:305:VAL:HG12	1.76	0.67
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.75	0.67
1:A:579:ARG:HB3	1:A:610:LEU:HD21	1.76	0.67
1:A:293:VAL:HG13	1:A:303:ILE:HD13	1.76	0.66
1:A:690:ARG:HE	1:A:694:PHE:HE1	1.42	0.66
1:A:955:THR:C	1:A:957:THR:H	2.01	0.66
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.25	0.66
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.60	0.66
1:A:629:GLN:HG2	1:A:1029:ILE:CD1	2.26	0.66
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.11	0.65
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.42	0.65
1:A:947:ARG:HH11	1:A:947:ARG:HB3	1.62	0.65
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.76	0.65
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.11	0.65
1:A:418:ILE:HG12	1:A:419:LYS:N	2.07	0.65
1:A:354:LEU:HA	1:A:527:ILE:O	1.96	0.64
1:A:625:GLY:O	1:A:629:GLN:HG3	1.97	0.64
1:A:360:LYS:HE2	1:A:419:LYS:HG2	1.80	0.64
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.25	0.64
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.79	0.64
1:A:687:ARG:HH11	1:A:687:ARG:HG3	1.61	0.64
1:A:995:MET:O	1:A:1005:HIS:HB2	1.98	0.63
1:A:315:LEU:O	1:A:726:THR:HG22	1.97	0.63
1:A:606:LYS:O	1:A:609:GLN:HB2	1.98	0.62
1:A:905:GLU:H	1:A:905:GLU:CD	2.06	0.62
1:A:602:GLU:CD	1:A:602:GLU:H	2.06	0.62
1:A:992:LEU:HA	1:A:995:MET:HE3	1.81	0.62
1:A:1060:ASN:ND2	1:A:1063:ASP:H	1.98	0.62
1:A:660:LEU:O	1:A:664:VAL:HG23	1.99	0.62
1:A:756:LYS:HA	1:A:756:LYS:HZ2	1.64	0.62
1:A:880:GLU:HG2	1:A:881:ILE:N	2.14	0.61
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.82	0.61
1:A:946:ASP:HB2	1:A:983:VAL:O	2.00	0.61
1:A:760:SER:O	1:A:763:VAL:HG12	2.01	0.61
1:A:531:LYS:HE2	1:A:605:ALA:HB2	1.83	0.60
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.15	0.60
1:A:370:ILE:HD13	1:A:371:PRO:N	2.15	0.60
1:A:784:ARG:HD3	1:A:789:PRO:O	2.02	0.60
1:A:806:SER:HB3	1:A:810:PRO:HD3	1.84	0.60
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.37	0.59
1:A:355:TRP:HH2	1:A:531:LYS:HG2	1.67	0.59
1:A:561:THR:O	1:A:591:LYS:NZ	2.35	0.59
1:A:1010:GLN:HB3	1:A:1069:LEU:HD21	1.84	0.59
1:A:162:VAL:HG21	1:A:718:GLU:OE2	2.03	0.59
1:A:567:LEU:HD22	1:A:571:ASP:HB3	1.85	0.59
1:A:547:MET:HE2	1:A:552:ARG:CA	2.33	0.59
1:A:198:MET:HE1	1:A:282:VAL:HG11	1.84	0.59
1:A:876:ILE:HD13	1:A:876:ILE:N	2.16	0.59
1:A:287:ILE:HD13	1:A:287:ILE:O	2.03	0.59
1:A:743:GLN:HG2	1:A:876:ILE:HG21	1.85	0.59
1:A:319:ARG:HG2	1:A:320:LYS:H	1.68	0.58
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.86	0.58
1:A:786:PRO:HD2	1:A:878:MET:HE1	1.84	0.58
1:A:784:ARG:CZ	1:A:792:LYS:HE3	2.33	0.58
1:A:861:ASP:C	1:A:862:LEU:HD22	2.28	0.58
1:A:389:HIS:O	1:A:392:GLN:HB3	2.04	0.58
1:A:359:ARG:HD2	1:A:360:LYS:H	1.69	0.58
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.85	0.57
1:A:402:LYS:HB3	1:A:403:PRO:HD2	1.86	0.57
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.34	0.57
1:A:750:LYS:HD3	1:A:751:SER:N	2.20	0.57
1:A:370:ILE:HD13	1:A:370:ILE:C	2.29	0.57
1:A:955:THR:C	1:A:957:THR:N	2.63	0.57
1:A:763:VAL:HA	1:A:766:GLN:HG3	1.85	0.57
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.87	0.57
1:A:622:LEU:HD12	1:A:623:ASP:N	2.20	0.56
1:A:738:VAL:HG21	1:A:783:PHE:HB3	1.87	0.56
1:A:174:GLU:O	1:A:178:ARG:HG3	2.05	0.56
1:A:914:LYS:O	1:A:916:PRO:HD3	2.06	0.56
1:A:497:PHE:CD1	1:A:1042:LEU:HB3	2.34	0.56
1:A:784:ARG:O	1:A:786:PRO:HD3	2.06	0.56
1:A:806:SER:C	1:A:808:LYS:H	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.69	0.56
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.41	0.56
1:A:564:LEU:HD13	1:A:1049:GLU:HA	1.87	0.56
1:A:687:ARG:HG3	1:A:687:ARG:NH1	2.21	0.55
1:A:563:PRO:HD3	1:A:1025:ASN:ND2	2.20	0.55
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.87	0.55
1:A:724:CYS:SG	1:A:729:LEU:HD13	2.47	0.55
1:A:1084:PHE:CE2	1:A:1088:LEU:HD11	2.41	0.55
1:A:1063:ASP:HA	1:A:1066:LYS:HE2	1.88	0.55
1:A:756:LYS:C	1:A:758:ASP:H	2.15	0.54
1:A:210:TYR:CE1	1:A:211:LEU:HG	2.42	0.54
1:A:1014:VAL:HG11	1:A:1065:LYS:CG	2.38	0.54
1:A:731:ASP:O	1:A:735:GLN:HG3	2.08	0.54
1:A:960:LEU:HG	1:A:961:PHE:N	2.22	0.54
1:A:464:VAL:HB	1:A:484:MET:HG2	1.90	0.54
1:A:847:ILE:O	1:A:850:ILE:HB	2.08	0.54
1:A:1045:LYS:H	1:A:1045:LYS:CD	2.12	0.54
1:A:735:GLN:O	1:A:739:ILE:HG12	2.08	0.54
1:A:834:HIS:HA	1:A:875:LYS:O	2.07	0.54
1:A:223:VAL:O	1:A:304:HIS:HA	2.07	0.54
1:A:386:ASN:OD1	1:A:396:GLN:HB2	2.08	0.54
1:A:913:GLU:HG3	1:A:914:LYS:N	2.22	0.54
1:A:364:LYS:NZ	1:A:411:ASN:O	2.41	0.53
1:A:953:MET:O	1:A:960:LEU:HD12	2.08	0.53
1:A:635:PHE:O	1:A:641:ARG:HD2	2.09	0.53
1:A:693:HIS:CD2	1:A:789:PRO:HB3	2.43	0.53
1:A:999:GLY:O	1:A:1000:LYS:HD3	2.08	0.53
1:A:846:GLN:O	1:A:850:ILE:HG12	2.09	0.53
1:A:306:VAL:HG13	1:A:308:ASP:OD1	2.08	0.52
1:A:732:PHE:O	1:A:736:VAL:HG23	2.09	0.52
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.90	0.52
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.92	0.52
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.52
1:A:360:LYS:CE	1:A:419:LYS:HG2	2.40	0.52
1:A:184:ARG:O	1:A:188:VAL:HG23	2.09	0.51
1:A:368:ILE:O	1:A:368:ILE:HG13	2.10	0.51
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.92	0.51
1:A:1045:LYS:O	1:A:1049:GLU:HG3	2.10	0.51
1:A:833:LYS:HG2	1:A:834:HIS:N	2.26	0.51
1:A:201:TRP:CZ3	1:A:690:ARG:NH1	2.79	0.51
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:GLN:HE22	1:A:902:PHE:HA	1.75	0.51
1:A:319:ARG:HG2	1:A:320:LYS:HG3	1.93	0.51
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.93	0.51
1:A:690:ARG:NE	1:A:694:PHE:HE1	2.06	0.51
1:A:702:GLU:O	1:A:706:SER:HB3	2.10	0.51
1:A:996:GLY:O	1:A:1001:LYS:HE3	2.10	0.51
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.40	0.51
1:A:428:LEU:C	1:A:428:LEU:HD23	2.36	0.51
1:A:464:VAL:HG11	1:A:516:ILE:HG21	1.93	0.51
1:A:470:ASP:OD1	1:A:472:ARG:N	2.40	0.51
1:A:1040:PRO:O	1:A:1041:GLN:C	2.54	0.51
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.92	0.50
1:A:955:THR:O	1:A:957:THR:N	2.44	0.50
1:A:434:TYR:HA	1:A:459:ARG:O	2.10	0.50
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.10	0.50
1:A:744:LYS:HE2	1:A:748:ASP:OD1	2.12	0.50
1:A:770:LYS:O	1:A:773:ASN:HB2	2.12	0.50
1:A:640:VAL:O	1:A:643:ILE:HG12	2.12	0.50
1:A:215:ILE:HG23	1:A:220:ILE:HG22	1.93	0.50
1:A:622:LEU:HD12	1:A:623:ASP:H	1.76	0.50
1:A:997:THR:HG22	1:A:997:THR:O	2.11	0.50
1:A:435:CYS:HB3	1:A:461:LEU:HD11	1.93	0.50
1:A:772:GLU:CG	1:A:798:ILE:HG12	2.42	0.50
1:A:935:TYR:O	1:A:939:THR:HG22	2.12	0.49
1:A:751:SER:C	1:A:753:SER:H	2.20	0.49
1:A:223:VAL:HB	1:A:304:HIS:CD2	2.47	0.49
1:A:614:ARG:HG3	1:A:618:ASP:OD2	2.13	0.49
1:A:900:GLY:HA2	1:A:902:PHE:CE2	2.47	0.49
1:A:1038:GLY:O	1:A:1040:PRO:HD3	2.12	0.49
1:A:233:ILE:N	1:A:233:ILE:HD12	2.27	0.49
1:A:652:GLU:HG2	1:A:655:ASP:OD2	2.13	0.49
1:A:271:VAL:HG22	1:A:272:LEU:N	2.28	0.49
1:A:435:CYS:SG	1:A:459:ARG:HG2	2.52	0.49
1:A:498:ASN:OD1	1:A:498:ASN:C	2.56	0.49
1:A:917:THR:HG23	1:A:920:LYS:HB2	1.93	0.49
1:A:951:ASN:HA	1:A:963:ILE:CD1	2.40	0.49
1:A:226:ARG:HD3	1:A:307:LEU:HB3	1.95	0.49
1:A:276:GLY:HA2	1:A:819:ASP:HB3	1.94	0.49
1:A:887:THR:HG22	1:A:889:ALA:H	1.77	0.49
1:A:364:LYS:HD3	1:A:519:LEU:HD23	1.94	0.49
1:A:1074:VAL:O	1:A:1078:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:O	1:A:244:ILE:HG13	2.12	0.48
1:A:873:GLY:HA3	1:A:876:ILE:HG12	1.94	0.48
1:A:633:CYS:SG	1:A:1036:MET:HE1	2.53	0.48
1:A:807:LYS:HD2	1:A:807:LYS:N	2.28	0.48
1:A:757:TYR:HB3	1:A:807:LYS:HG3	1.95	0.48
1:A:803:VAL:HG22	1:A:811:LEU:CD2	2.43	0.48
1:A:484:MET:HE3	1:A:516:ILE:HG21	1.96	0.48
1:A:705:GLN:OE1	1:A:839:ARG:NE	2.46	0.48
1:A:219:CYS:HA	1:A:236:SER:HA	1.95	0.47
1:A:738:VAL:HG22	1:A:780:PRO:HD2	1.96	0.47
1:A:187:GLU:CD	1:A:687:ARG:HG2	2.39	0.47
1:A:625:GLY:HA2	1:A:1026:LEU:HD23	1.96	0.47
1:A:287:ILE:HD13	1:A:287:ILE:C	2.40	0.47
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.42	0.47
1:A:927:ARG:HE	1:A:959:ASN:ND2	2.11	0.47
1:A:222:ILE:HG13	1:A:222:ILE:O	2.15	0.47
1:A:483:HIS:CD2	1:A:510:LYS:HG2	2.50	0.47
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.49	0.47
1:A:477:ARG:HD3	1:A:521:ASP:O	2.15	0.47
1:A:547:MET:HE3	1:A:551:LEU:HB3	1.97	0.47
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.97	0.47
1:A:810:PRO:O	1:A:811:LEU:HD23	2.14	0.47
1:A:474:LEU:HD22	1:A:527:ILE:HG12	1.96	0.47
1:A:652:GLU:O	1:A:656:VAL:HG23	2.15	0.47
1:A:390:GLY:C	1:A:392:GLN:H	2.23	0.46
1:A:806:SER:C	1:A:808:LYS:N	2.73	0.46
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.15	0.46
1:A:292:TRP:O	1:A:295:HIS:HB3	2.14	0.46
1:A:477:ARG:HD2	1:A:478:GLY:H	1.80	0.46
1:A:552:ARG:O	1:A:556:GLU:HG3	2.15	0.46
1:A:308:ASP:OD1	1:A:308:ASP:N	2.48	0.46
1:A:662:GLN:NE2	1:A:1030:LEU:HD22	2.31	0.46
1:A:164:ASP:C	1:A:166:SER:H	2.24	0.46
1:A:987:LEU:CD1	1:A:995:MET:HE1	2.32	0.46
1:A:997:THR:HG21	1:A:1076:ARG:NH2	2.30	0.46
1:A:418:ILE:HD13	1:A:423:LEU:HD23	1.98	0.46
1:A:807:LYS:HD2	1:A:807:LYS:H	1.80	0.46
1:A:984:PRO:HB2	1:A:985:PHE:CD2	2.50	0.46
1:A:628:MET:HE3	1:A:1030:LEU:HD21	1.98	0.46
1:A:988:THR:O	1:A:991:PHE:HB2	2.15	0.46
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ARG:HG3	1:A:227:SER:H	1.80	0.46
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.50	0.46
1:A:547:MET:HE2	1:A:552:ARG:N	2.31	0.46
1:A:1041:GLN:O	1:A:1043:THR:N	2.49	0.46
1:A:581:GLU:OE2	1:A:584:LYS:HD2	2.16	0.45
1:A:707:ARG:HD2	1:A:710:GLN:OE1	2.16	0.45
1:A:963:ILE:O	1:A:964:ASP:C	2.59	0.45
1:A:520:LEU:O	1:A:521:ASP:C	2.59	0.45
1:A:725:GLY:O	1:A:729:LEU:HB2	2.15	0.45
1:A:1041:GLN:HE21	1:A:1041:GLN:N	2.14	0.45
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.47	0.45
1:A:622:LEU:HD21	1:A:651:LEU:HG	1.98	0.45
1:A:945:GLY:C	1:A:985:PHE:HA	2.41	0.45
1:A:523:TYR:HB3	1:A:524:CYS:H	1.48	0.45
1:A:1035:LEU:C	1:A:1043:THR:HG21	2.41	0.45
1:A:212:TRP:CE3	1:A:212:TRP:HA	2.51	0.45
1:A:548:PRO:HB2	1:A:551:LEU:HB2	1.99	0.45
1:A:775:GLN:OE1	1:A:779:LEU:HD23	2.16	0.45
1:A:983:VAL:HB	1:A:1082:VAL:HG21	1.99	0.45
1:A:696:PHE:CE1	1:A:721:LEU:HD21	2.51	0.45
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.80	0.45
1:A:319:ARG:HG2	1:A:320:LYS:N	2.29	0.45
1:A:559:ILE:HD13	1:A:588:ALA:HB2	1.97	0.45
1:A:729:LEU:HD12	1:A:729:LEU:HA	1.67	0.45
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.17	0.45
1:A:1052:ARG:HD3	1:A:1057:VAL:HG21	1.99	0.45
1:A:779:LEU:HD12	1:A:780:PRO:HD2	1.98	0.45
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.98	0.45
1:A:907:LEU:HD12	1:A:990:ASP:OD2	2.17	0.45
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.51	0.45
1:A:1060:ASN:HD22	1:A:1062:GLU:HB2	1.81	0.45
1:A:555:LEU:O	1:A:559:ILE:HG13	2.17	0.44
1:A:1078:LYS:O	1:A:1079:GLY:C	2.60	0.44
1:A:174:GLU:HA	1:A:177:ARG:HD3	1.99	0.44
1:A:803:VAL:HG13	1:A:810:PRO:O	2.17	0.44
1:A:851:MET:HE2	1:A:1020:LEU:HD13	1.98	0.44
1:A:212:TRP:HA	1:A:212:TRP:HE3	1.83	0.44
1:A:1076:ARG:HB3	1:A:1076:ARG:NH1	2.28	0.44
1:A:293:VAL:HG13	1:A:303:ILE:CD1	2.44	0.44
1:A:589:TYR:HB2	1:A:590:PRO:HD3	2.00	0.44
1:A:667:VAL:O	1:A:712:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:ARG:HH11	1:A:947:ARG:CB	2.29	0.44
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.53	0.44
1:A:745:VAL:O	1:A:749:ILE:HG12	2.18	0.44
1:A:838:LEU:CD1	1:A:877:GLY:HA3	2.43	0.44
1:A:244:ILE:HG22	1:A:245:LEU:H	1.83	0.44
1:A:470:ASP:OD1	1:A:470:ASP:C	2.60	0.44
1:A:281:LEU:HD22	1:A:290:PHE:CD2	2.53	0.43
1:A:755:GLU:C	1:A:756:LYS:HZ3	2.26	0.43
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.83	0.43
1:A:862:LEU:HD12	1:A:934:GLY:N	2.33	0.43
1:A:933:ALA:O	1:A:937:VAL:HG23	2.19	0.43
1:A:1024:THR:O	1:A:1028:ILE:HG13	2.18	0.43
1:A:360:LYS:HE2	1:A:419:LYS:HE2	1.99	0.43
1:A:657:LEU:HG	1:A:691:ILE:HG12	2.00	0.43
1:A:765:SER:O	1:A:769:GLN:HB2	2.19	0.43
1:A:946:ASP:OD1	1:A:983:VAL:HG12	2.18	0.43
1:A:561:THR:HG22	1:A:562:ASP:N	2.33	0.43
1:A:784:ARG:NH2	1:A:792:LYS:HE3	2.32	0.43
1:A:863:CYS:HB3	1:A:959:ASN:HD21	1.82	0.43
1:A:988:THR:HG21	1:A:1083:GLN:HG3	2.00	0.43
1:A:887:THR:O	1:A:891:ILE:HG13	2.18	0.43
1:A:271:VAL:HG23	1:A:282:VAL:HG13	2.01	0.43
1:A:892:GLN:NE2	1:A:902:PHE:HA	2.33	0.43
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.19	0.43
1:A:221:PHE:CE1	1:A:234:LYS:HG2	2.29	0.43
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.53	0.43
1:A:853:SER:O	1:A:857:THR:HG23	2.19	0.43
1:A:917:THR:OG1	1:A:919:GLU:HB3	2.19	0.43
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.82	0.43
1:A:150:PHE:O	1:A:153:GLN:HB3	2.19	0.43
1:A:497:PHE:CB	1:A:1042:LEU:HD22	2.33	0.43
1:A:390:GLY:N	1:A:636:SER:HB3	2.34	0.43
1:A:531:LYS:HE2	1:A:605:ALA:CB	2.49	0.43
1:A:525:HIS:N	1:A:526:PRO:HD3	2.35	0.42
1:A:576:TRP:O	1:A:577:HIS:C	2.62	0.42
1:A:198:MET:CE	1:A:282:VAL:HG21	2.48	0.42
1:A:382:PHE:CE1	1:A:434:TYR:HB2	2.55	0.42
1:A:390:GLY:C	1:A:392:GLN:N	2.78	0.42
1:A:863:CYS:SG	1:A:927:ARG:HD3	2.59	0.42
1:A:1014:VAL:HG13	1:A:1065:LYS:HA	2.01	0.42
1:A:309:THR:HG22	1:A:310:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:LYS:HE2	1:A:501:LYS:HB3	1.83	0.42
1:A:983:VAL:HG22	1:A:984:PRO:CD	2.45	0.42
1:A:997:THR:HG23	1:A:1001:LYS:HG3	2.00	0.42
1:A:370:ILE:O	1:A:370:ILE:HG23	2.19	0.42
1:A:831:ILE:CG2	1:A:832:PHE:N	2.83	0.42
1:A:918:GLU:O	1:A:922:GLN:HG2	2.19	0.42
1:A:162:VAL:O	1:A:177:ARG:NH1	2.53	0.42
1:A:275:CYS:SG	1:A:821:THR:HG22	2.60	0.42
1:A:685:GLY:C	1:A:687:ARG:N	2.78	0.42
1:A:947:ARG:CB	1:A:947:ARG:NH1	2.83	0.42
1:A:382:PHE:CZ	1:A:434:TYR:HB2	2.55	0.42
1:A:829:GLY:HA3	1:A:881:ILE:HB	2.03	0.41
1:A:682:LEU:HD21	1:A:720:TYR:HA	2.02	0.41
1:A:766:GLN:HE21	1:A:766:GLN:HB3	1.56	0.41
1:A:400:SER:HA	1:A:401:PRO:HD3	1.88	0.41
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.95	0.41
1:A:531:LYS:HD2	1:A:608:TYR:CD1	2.46	0.41
1:A:720:TYR:CZ	1:A:724:CYS:HB3	2.55	0.41
1:A:844:ILE:O	1:A:848:LEU:HD13	2.21	0.41
1:A:889:ALA:O	1:A:893:GLN:HG3	2.20	0.41
1:A:904:ASP:OD2	1:A:904:ASP:N	2.52	0.41
1:A:239:ASP:O	1:A:286:PRO:HA	2.20	0.41
1:A:775:GLN:HE22	1:A:796:LEU:H	1.68	0.41
1:A:845:LEU:HD12	1:A:845:LEU:HA	1.84	0.41
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.20	0.41
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.51	0.41
1:A:749:ILE:HG21	1:A:803:VAL:HG21	2.03	0.41
1:A:1076:ARG:C	1:A:1078:LYS:H	2.28	0.41
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.55	0.41
1:A:696:PHE:CD1	1:A:721:LEU:HD21	2.56	0.41
1:A:764:ILE:O	1:A:768:LYS:HG3	2.21	0.41
1:A:862:LEU:HD13	1:A:862:LEU:HA	1.88	0.41
1:A:632:ASP:OD1	1:A:634:ASN:HB2	2.20	0.41
1:A:720:TYR:CD2	1:A:720:TYR:C	2.99	0.41
1:A:823:LEU:HD22	1:A:823:LEU:H	1.86	0.41
1:A:180:LEU:C	1:A:183:PRO:HD2	2.46	0.41
1:A:286:PRO:O	1:A:289:ASN:HB2	2.20	0.41
1:A:370:ILE:HD13	1:A:372:VAL:N	2.36	0.41
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.94	0.41
1:A:418:ILE:CG1	1:A:419:LYS:H	2.16	0.41
1:A:550:GLN:O	1:A:550:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:HA	1:A:551:LEU:HD12	1.72	0.41
1:A:643:ILE:O	1:A:647:LYS:HG2	2.21	0.41
1:A:663:LEU:O	1:A:664:VAL:C	2.63	0.41
1:A:1032:SER:O	1:A:1036:MET:HG2	2.20	0.41
1:A:354:LEU:HD23	1:A:354:LEU:N	2.36	0.40
1:A:477:ARG:HG3	1:A:478:GLY:N	2.36	0.40
1:A:637:ASP:OD1	1:A:639:ASN:HB2	2.21	0.40
1:A:806:SER:HB3	1:A:810:PRO:CD	2.51	0.40
1:A:1027:LEU:HD12	1:A:1027:LEU:HA	1.78	0.40
1:A:1053:ASP:OD1	1:A:1053:ASP:N	2.53	0.40
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.84	0.40
1:A:796:LEU:HB3	1:A:797:ALA:H	1.65	0.40
1:A:996:GLY:O	1:A:1003:SER:HB3	2.21	0.40
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.51	0.40
1:A:711:GLN:O	1:A:712:ARG:C	2.65	0.40
1:A:741:MET:O	1:A:744:LYS:HB3	2.21	0.40
1:A:773:ASN:HA	1:A:776:ASN:ND2	2.37	0.40
1:A:944:ILE:HD12	1:A:965:PHE:HD2	1.87	0.40
1:A:245:LEU:CA	1:A:248:PHE:HB3	2.52	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	830/966 (86%)	690 (83%)	115 (14%)	25 (3%)	3 8

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	916	PRO
1	A	165	VAL

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Mol	Chain	Res	Type
1	A	214	LYS
1	A	251	LYS
1	A	776	ASN
1	A	956	GLU
1	A	1042	LEU
1	A	226	ARG
1	A	239	ASP
1	A	752	LEU
1	A	796	LEU
1	A	216	ALA
1	A	354	LEU
1	A	757	TYR
1	A	874	ASP
1	A	162	VAL
1	A	425	LYS
1	A	896	VAL
1	A	964	ASP
1	A	418	ILE
1	A	798	ILE
1	A	906	VAL
1	A	1079	GLY
1	A	759	VAL
1	A	780	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	761/864 (88%)	696 (92%)	65 (8%)	10 22

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	202	VAL
1	A	245	LEU

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Mol	Chain	Res	Type
1	A	246	GLN
1	A	249	PHE
1	A	282	VAL
1	A	285	THR
1	A	287	ILE
1	A	309	THR
1	A	320	LYS
1	A	354	LEU
1	A	357	CYS
1	A	360	LYS
1	A	370	ILE
1	A	372	VAL
1	A	381	VAL
1	A	391	GLN
1	A	395	CYS
1	A	396	GLN
1	A	410	TRP
1	A	417	SER
1	A	471	HIS
1	A	477	ARG
1	A	482	LEU
1	A	516	ILE
1	A	524	CYS
1	A	525	HIS
1	A	546	GLU
1	A	550	GLN
1	A	551	LEU
1	A	575	LEU
1	A	601	GLN
1	A	613	ARG
1	A	626	LEU
1	A	636	SER
1	A	682	LEU
1	A	687	ARG
1	A	717	LEU
1	A	729	LEU
1	A	750	LYS
1	A	756	LYS
1	A	766	GLN
1	A	814	GLU
1	A	843	LEU
1	A	845	LEU

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Mol	Chain	Res	Type
1	A	847	ILE
1	A	858	GLU
1	A	860	LEU
1	A	874	ASP
1	A	876	ILE
1	A	904	ASP
1	A	905	GLU
1	A	913	GLU
1	A	917	THR
1	A	919	GLU
1	A	947	ARG
1	A	953	MET
1	A	957	THR
1	A	960	LEU
1	A	1024	THR
1	A	1026	LEU
1	A	1027	LEU
1	A	1037	THR
1	A	1041	GLN
1	A	1076	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	153	GLN
1	A	218	ASN
1	A	225	HIS
1	A	388	GLN
1	A	391	GLN
1	A	396	GLN
1	A	432	GLN
1	A	483	HIS
1	A	550	GLN
1	A	577	HIS
1	A	619	GLN
1	A	634	ASN
1	A	705	GLN
1	A	708	HIS
1	A	711	GLN
1	A	734	GLN
1	A	737	GLN

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Mol	Chain	Res	Type
1	A	766	GLN
1	A	776	ASN
1	A	825	ASN
1	A	840	GLN
1	A	892	GLN
1	A	949	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1010	GLN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN
1	A	1089	HIS

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	41A	A	2040	-	20,20,20	0.91	2 (10%)	27,30,30	1.20	3 (11%)

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	41A	A	2040	-	-	2/4/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2040	41A	C04-C02	2.45	1.57	1.53
2	A	2040	41A	C08-C02	2.05	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2040	41A	C17-N12-C11	-3.87	112.29	122.09
2	A	2040	41A	C02-C08-C07	2.47	118.32	114.44
2	A	2040	41A	C13-N12-C11	-2.41	115.97	122.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

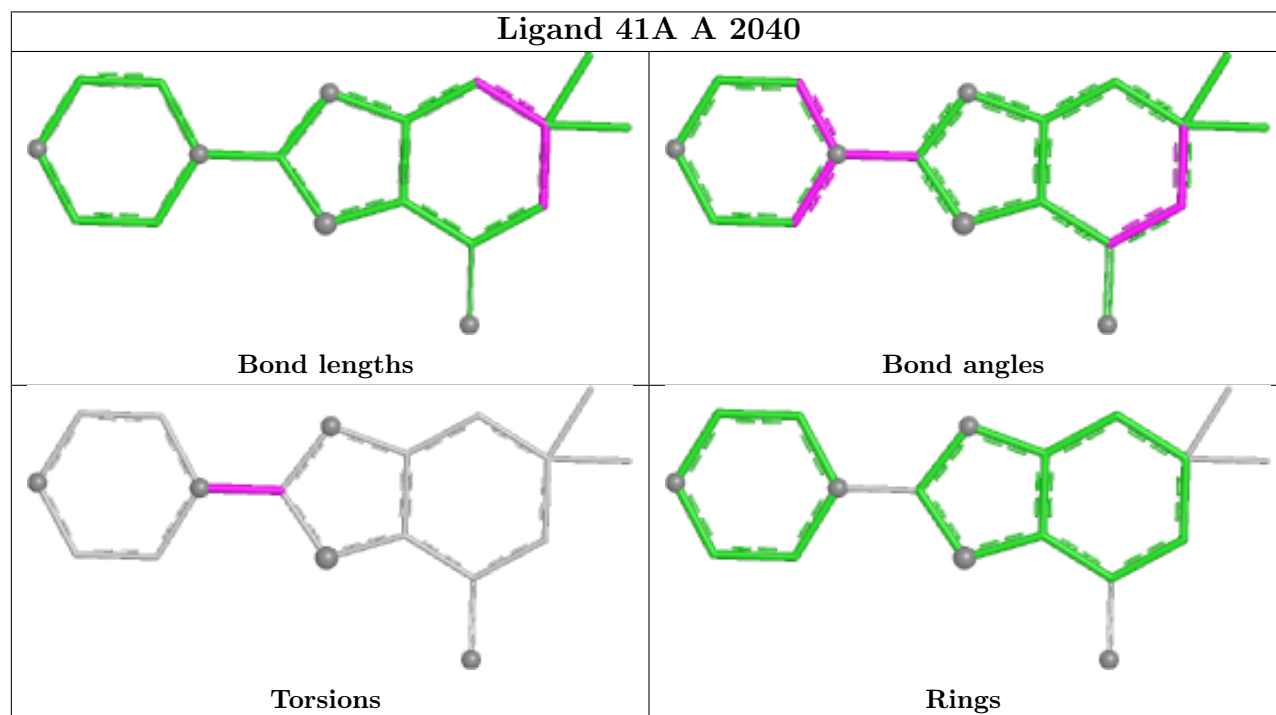
Mol	Chain	Res	Type	Atoms
2	A	2040	41A	S10-C11-N12-C13
2	A	2040	41A	N18-C11-N12-C13

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

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	846/966 (87%)	0.11	23 (2%)	56 47	14, 58, 106, 126	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	TYR	3.3
1	A	211	LEU	2.9
1	A	1042	LEU	2.9
1	A	352	VAL	2.8
1	A	995	MET	2.7
1	A	528	ALA	2.6
1	A	756	LYS	2.5
1	A	252	MET	2.5
1	A	779	LEU	2.2
1	A	249	PHE	2.2
1	A	754	ALA	2.2
1	A	823	LEU	2.2
1	A	892	GLN	2.2
1	A	1090	LEU	2.2
1	A	527	ILE	2.1
1	A	379	LEU	2.1
1	A	1091	VAL	2.1
1	A	525	HIS	2.1
1	A	948	HIS	2.1
1	A	208	PRO	2.1
1	A	1064	ALA	2.1
1	A	532	HIS	2.0
1	A	216	ALA	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](#)

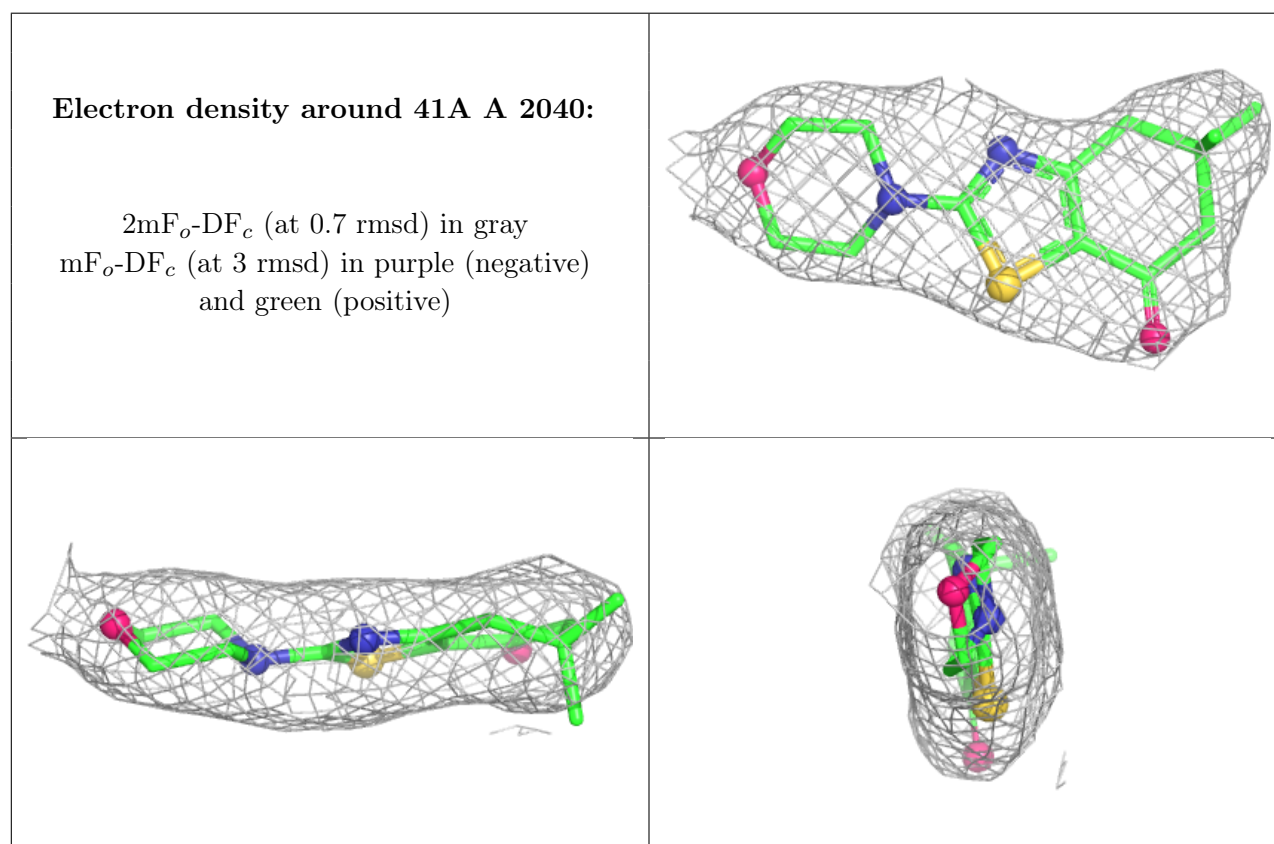
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	41A	A	2040	18/18	0.95	0.09	49,60,66,70	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.