



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:14 AM UTC

PDB ID : 1E8W / pdb_00001e8w
Title : Structure determinants of phosphoinositide 3-kinase inhibition by wortmannin, LY294002, quercetin, myricetin and staurosporine
Authors : Walker, E.H.; Pacold, M.E.; Perisic, O.; Stephens, L.; Hawkins, P.T.; Wymann, M.P.; Williams, R.L.
Deposited on : 2000-10-03
Resolution : 2.50 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

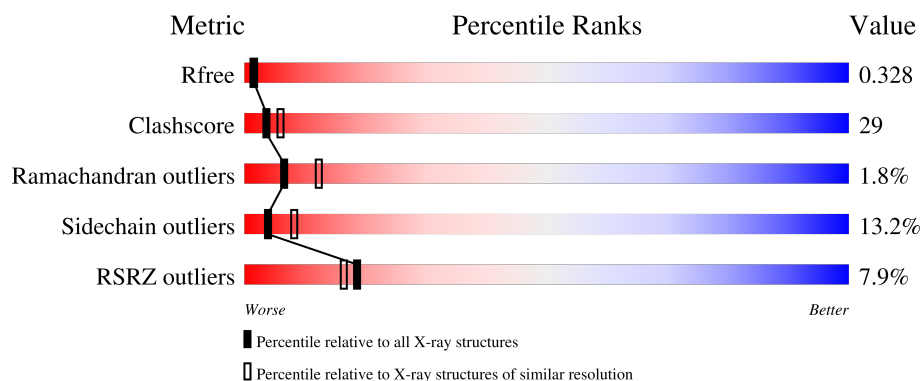
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	961	

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	QUE	A	2095	-	X	-	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6915 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.

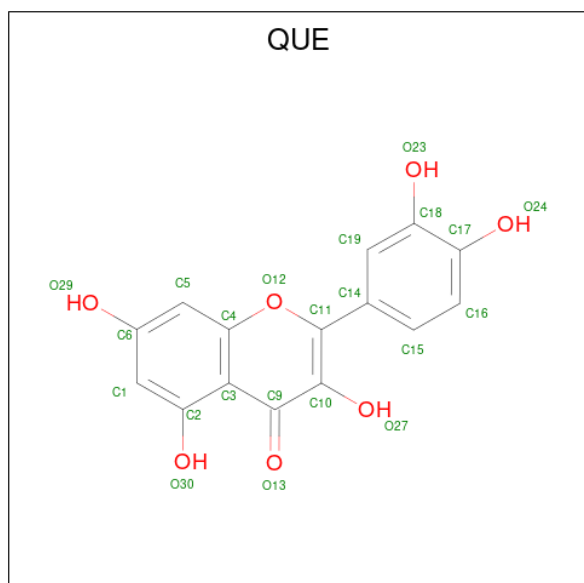
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	851	6893	4435	1167	1254	37	0	0	0

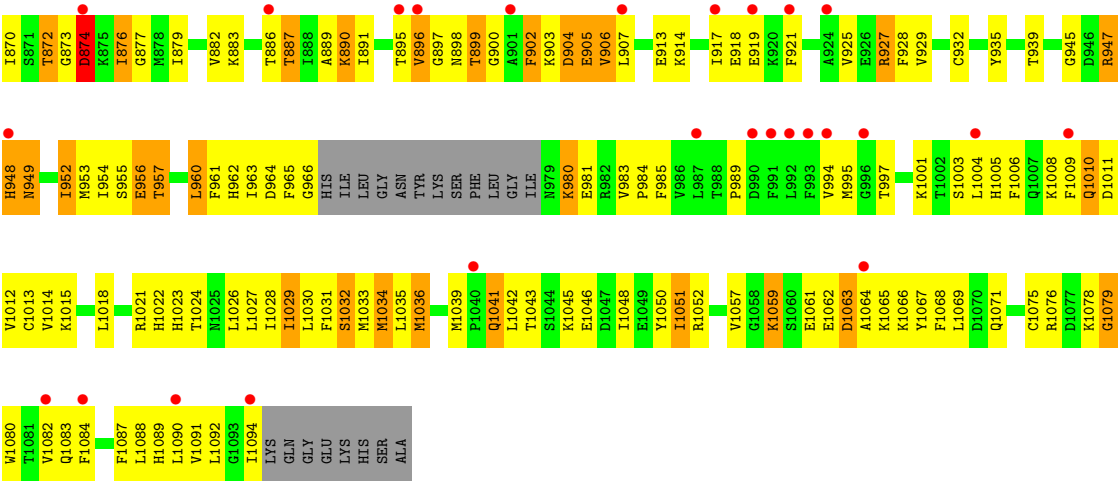
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ALA	PRO	expression tag	UNP O02697
A	505	ALA	ARG	conflict	UNP O02697

- Molecule 2 is 3,5,7,3',4'-PENTAHYDROXYFLAVONE (CCD ID: QUE) (formula: C₁₅H₁₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	22	15	7	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.16Å 67.44Å 106.70Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	62.45 – 2.50 62.45 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.4 (62.45-2.50) 98.5 (62.45-2.51)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.265 , 0.330 0.262 , 0.328	Depositor DCC
R_{free} test set	1706 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	62.2	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6915	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: QUE

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	1.19	26/7039 (0.4%)	1.26	38/9524 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	842	MET	SD-CE	-12.10	1.49	1.79
1	A	198	MET	SD-CE	10.04	2.04	1.79
1	A	804	MET	SD-CE	-7.87	1.59	1.79
1	A	507	ASN	CA-C	7.50	1.61	1.52
1	A	844	ILE	CA-CB	7.47	1.63	1.54
1	A	691	ILE	CA-CB	-7.45	1.45	1.54
1	A	514	MET	SD-CE	7.30	1.97	1.79
1	A	664	VAL	CA-CB	6.87	1.63	1.54
1	A	715	VAL	CA-CB	6.84	1.64	1.54
1	A	739	ILE	CA-CB	-6.74	1.45	1.54
1	A	829	GLY	CA-C	-6.72	1.47	1.52
1	A	676	ALA	N-CA	-6.47	1.38	1.46
1	A	882	VAL	CA-CB	-6.13	1.46	1.54
1	A	383	VAL	CA-CB	-6.02	1.46	1.54
1	A	675	SER	CA-C	-6.01	1.45	1.52
1	A	182	THR	CA-CB	5.93	1.61	1.53
1	A	499	ALA	CA-CB	-5.37	1.44	1.53
1	A	712	ARG	CA-C	-5.35	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	TYR	N-CA	5.28	1.52	1.45
1	A	1032	SER	CA-C	5.23	1.59	1.52
1	A	431	LEU	N-CA	5.23	1.52	1.46
1	A	168	VAL	CA-CB	-5.21	1.46	1.55
1	A	1034	MET	N-CA	-5.17	1.40	1.46
1	A	503	THR	CA-C	-5.14	1.46	1.52
1	A	872	THR	CA-CB	-5.07	1.46	1.53
1	A	882	VAL	CA-C	-5.02	1.47	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	THR	N-CA-C	-8.55	100.38	113.89
1	A	670	GLU	CA-C-N	-8.51	110.97	119.56
1	A	670	GLU	C-N-CA	-8.51	110.97	119.56
1	A	484	MET	N-CA-C	8.27	122.75	110.52
1	A	373	LEU	CA-C-N	7.65	127.64	119.76
1	A	373	LEU	C-N-CA	7.65	127.64	119.76
1	A	357	CYS	N-CA-C	-7.32	95.22	110.80
1	A	847	ILE	N-CA-C	-7.26	103.21	110.62
1	A	243	THR	N-CA-C	-7.20	103.51	111.36
1	A	503	THR	N-CA-C	7.08	119.98	110.35
1	A	499	ALA	N-CA-C	6.86	119.63	111.33
1	A	839	ARG	N-CA-C	-6.77	103.97	111.82
1	A	906	VAL	N-CA-C	6.67	117.36	110.36
1	A	595	SER	N-CA-C	-6.66	104.90	113.16
1	A	606	LYS	N-CA-C	-6.55	104.22	111.36
1	A	863	CYS	N-CA-C	6.53	120.52	111.90
1	A	169	HIS	N-CA-C	-6.47	103.81	112.94
1	A	858	GLU	N-CA-C	-6.29	105.98	113.21
1	A	158	ILE	CB-CA-C	-6.22	103.64	112.22
1	A	673	HIS	CA-C-N	-5.86	114.63	122.72
1	A	673	HIS	C-N-CA	-5.86	114.63	122.72
1	A	785	VAL	N-CA-C	-5.58	102.13	107.76
1	A	234	LYS	N-CA-C	-5.53	100.28	109.46
1	A	948	HIS	CA-C-N	5.50	128.20	120.28
1	A	948	HIS	C-N-CA	5.50	128.20	120.28
1	A	695	LEU	N-CA-C	-5.39	105.49	111.36
1	A	504	SER	N-CA-C	-5.36	106.33	112.92
1	A	902	PHE	N-CA-C	5.33	118.04	110.10
1	A	745	VAL	CB-CA-C	-5.33	105.15	111.97
1	A	547	MET	N-CA-C	5.27	112.96	108.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	VAL	N-CA-C	5.25	117.41	108.86
1	A	239	ASP	N-CA-C	5.24	117.79	109.24
1	A	874	ASP	CA-C-N	-5.15	115.50	123.17
1	A	874	ASP	C-N-CA	-5.15	115.50	123.17
1	A	660	LEU	N-CA-C	5.14	116.74	111.03
1	A	223	VAL	CB-CA-C	-5.09	105.73	111.23
1	A	562	ASP	CA-C-N	5.04	124.64	119.05
1	A	562	ASP	C-N-CA	5.04	124.64	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	693	HIS	Sidechain
1	A	720	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6893	0	6963	407	0
2	A	22	0	10	4	0
All	All	6915	0	6973	407	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 29.

All (407) 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:198:MET:SD	1:A:198:MET:CE	2.04	1.44
1:A:807:LYS:H	1:A:807:LYS:HD2	1.18	1.02
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.37	1.01
1:A:299:ASN:HB3	1:A:301:GLU:HG3	1.42	0.99
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:O	1:A:614:ARG:HG3	1.64	0.95
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.46	0.94
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.49	0.93
1:A:576:TRP:O	1:A:579:ARG:HG3	1.69	0.92
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.53	0.90
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.51	0.90
1:A:887:THR:HG22	1:A:890:LYS:H	1.38	0.88
1:A:1084:PHE:CE2	1:A:1088:LEU:HD11	2.10	0.86
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.61	0.82
1:A:547:MET:HE2	1:A:552:ARG:HA	1.60	0.82
1:A:1018:LEU:HD22	1:A:1061:GLU:HG2	1.59	0.82
1:A:927:ARG:HG2	1:A:927:ARG:HH11	1.41	0.82
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.15	0.81
1:A:584:LYS:O	1:A:616:VAL:HG11	1.81	0.80
1:A:211:LEU:HD21	1:A:298:LYS:HB2	1.63	0.80
1:A:741:MET:HE2	1:A:774:LEU:HD22	1.64	0.80
1:A:150:PHE:O	1:A:153:GLN:HG2	1.81	0.79
1:A:1045:LYS:H	1:A:1045:LYS:HD2	1.47	0.79
1:A:153:GLN:HG3	1:A:154:LEU:HD23	1.65	0.78
1:A:760:SER:O	1:A:763:VAL:HG12	1.84	0.77
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.65	0.77
1:A:842:MET:HE3	1:A:870:ILE:HA	1.68	0.76
1:A:687:ARG:HH11	1:A:687:ARG:HG3	1.49	0.76
1:A:827:THR:O	1:A:883:LYS:HE2	1.86	0.76
1:A:405:THR:HG22	1:A:408:VAL:HG22	1.66	0.76
1:A:354:LEU:HB3	1:A:529:LEU:HD11	1.67	0.75
1:A:303:ILE:HG22	1:A:305:LEU:HD21	1.67	0.75
1:A:1041:GLN:H	1:A:1041:GLN:HE21	1.33	0.74
1:A:747:ILE:HD11	1:A:876:ILE:CD1	2.18	0.74
1:A:464:VAL:HB	1:A:484:MET:HG2	1.71	0.73
1:A:798:ILE:HD12	1:A:798:ILE:H	1.54	0.72
1:A:747:ILE:HD11	1:A:876:ILE:HD11	1.70	0.72
1:A:364:LYS:NZ	1:A:411:ASN:OD1	2.21	0.72
1:A:175:PHE:CZ	1:A:179:ARG:HD2	2.25	0.71
1:A:622:LEU:HD13	1:A:647:LYS:O	1.89	0.71
1:A:947:ARG:HH11	1:A:947:ARG:HB3	1.54	0.71
1:A:547:MET:HE2	1:A:552:ARG:CA	2.20	0.71
1:A:180:LEU:C	1:A:183:PRO:HD2	2.16	0.70
1:A:927:ARG:HG2	1:A:927:ARG:NH1	2.07	0.70
1:A:1024:THR:O	1:A:1028:ILE:HG12	1.92	0.70
1:A:842:MET:HE3	1:A:870:ILE:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:TRP:HB3	1:A:412:VAL:HG23	1.72	0.70
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.22	0.70
1:A:755:GLU:O	1:A:756:LYS:HE2	1.92	0.69
1:A:398:ARG:O	1:A:414:LEU:HD21	1.91	0.69
1:A:842:MET:CE	1:A:870:ILE:HD13	2.22	0.69
1:A:1010:GLN:O	1:A:1014:VAL:HG23	1.92	0.69
1:A:889:ALA:HB2	1:A:949:ASN:HB3	1.75	0.69
1:A:907:LEU:HD22	1:A:994:VAL:HG21	1.72	0.69
1:A:299:ASN:O	1:A:301:GLU:HG2	1.94	0.68
1:A:1088:LEU:HD23	1:A:1092:LEU:HD12	1.76	0.68
1:A:472:ARG:O	1:A:473:PHE:HB2	1.95	0.67
1:A:184:ARG:O	1:A:188:VAL:HG23	1.94	0.67
1:A:146:GLU:HG2	1:A:319:ARG:HH12	1.59	0.67
1:A:466:LEU:HD11	1:A:476:ARG:CD	2.21	0.67
1:A:362:ARG:NH2	1:A:413:TRP:CZ2	2.62	0.67
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.77	0.66
1:A:274:VAL:HG11	1:A:292:TRP:CE2	2.30	0.66
1:A:487:LEU:HD23	1:A:488:SER:N	2.10	0.66
1:A:734:GLN:O	1:A:738:VAL:HG23	1.96	0.66
1:A:418:ILE:HG13	1:A:419:LYS:N	2.07	0.65
1:A:154:LEU:HD23	1:A:154:LEU:N	2.12	0.65
1:A:379:LEU:O	1:A:403:PRO:HA	1.97	0.65
1:A:895:THR:HG21	1:A:906:VAL:HG22	1.79	0.65
1:A:221:PHE:CE1	1:A:234:LYS:HG2	2.31	0.65
1:A:379:LEU:HD12	1:A:404:PHE:HD2	1.62	0.65
1:A:689:LYS:HG2	1:A:728:MET:CE	2.26	0.65
1:A:682:LEU:HD22	1:A:686:LEU:CD1	2.27	0.65
1:A:775:GLN:O	1:A:775:GLN:HG3	1.97	0.65
1:A:955:SER:C	1:A:957:THR:H	2.04	0.64
1:A:611:LEU:HD22	1:A:614:ARG:HD3	1.78	0.64
1:A:405:THR:HG23	1:A:407:GLU:H	1.62	0.64
1:A:547:MET:HG2	1:A:552:ARG:NH2	2.12	0.64
1:A:565:ASN:OD1	1:A:566:PRO:HD2	1.98	0.64
1:A:1041:GLN:H	1:A:1041:GLN:NE2	1.96	0.64
1:A:370:ILE:HG23	1:A:370:ILE:O	1.97	0.64
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.79	0.64
1:A:487:LEU:HD23	1:A:488:SER:H	1.63	0.64
1:A:180:LEU:O	1:A:183:PRO:HD2	1.98	0.64
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.33	0.64
1:A:808:LYS:HE2	1:A:836:ASP:OD1	1.98	0.63
1:A:273:ARG:NH1	1:A:308:ASP:OD2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ARG:O	1:A:520:LEU:HD23	1.98	0.63
1:A:236:SER:OG	1:A:239:ASP:HB2	1.99	0.63
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.81	0.63
1:A:232:THR:C	1:A:233:ILE:HD12	2.24	0.63
1:A:240:THR:C	1:A:242:GLY:H	2.07	0.62
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.79	0.62
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.81	0.62
1:A:807:LYS:H	1:A:807:LYS:CD	1.98	0.62
1:A:739:ILE:O	1:A:743:GLN:HG3	1.99	0.62
1:A:921:PHE:O	1:A:925:VAL:HG23	1.98	0.62
1:A:498:ASN:OD1	1:A:498:ASN:C	2.41	0.62
1:A:601:GLN:HE21	1:A:602:GLU:HA	1.65	0.62
1:A:1064:ALA:O	1:A:1065:LYS:C	2.43	0.62
1:A:244:ILE:O	1:A:245:LEU:HB2	2.00	0.61
1:A:550:GLN:OE1	1:A:550:GLN:HA	1.98	0.61
1:A:737:GLN:O	1:A:741:MET:HG3	1.99	0.61
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.15	0.61
1:A:181:VAL:CG1	1:A:185:MET:HE2	2.24	0.61
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.18	0.61
1:A:233:ILE:HD12	1:A:233:ILE:N	2.16	0.61
1:A:150:PHE:HD1	1:A:153:GLN:NE2	1.99	0.61
1:A:743:GLN:O	1:A:747:ILE:HD12	2.01	0.60
1:A:561:THR:HG21	1:A:565:ASN:CG	2.27	0.60
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.35	0.60
1:A:707:ARG:HG3	1:A:710:GLN:OE1	2.02	0.59
1:A:899:THR:HA	1:A:1087:PHE:CZ	2.37	0.59
1:A:804:MET:HE1	1:A:831:ILE:HD13	1.84	0.59
1:A:855:TRP:CE3	1:A:862:LEU:HD23	2.37	0.59
1:A:855:TRP:CD2	1:A:862:LEU:HD23	2.37	0.59
1:A:657:LEU:HD11	1:A:690:ARG:HD3	1.85	0.59
1:A:807:LYS:HD2	1:A:807:LYS:N	2.02	0.59
1:A:953:MET:HE1	2:A:2095:QUE:C1	2.33	0.59
1:A:1011:ASP:O	1:A:1015:LYS:HB2	2.01	0.59
1:A:1048:ILE:O	1:A:1051:ILE:HG22	2.03	0.58
1:A:150:PHE:HA	1:A:153:GLN:HE21	1.67	0.58
1:A:244:ILE:HD12	1:A:244:ILE:H	1.68	0.58
1:A:281:LEU:HD22	1:A:290:PHE:CD2	2.38	0.58
1:A:497:PHE:HB2	1:A:1042:LEU:HD13	1.83	0.58
1:A:549:ASN:H	1:A:549:ASN:HD22	1.51	0.58
1:A:547:MET:CG	1:A:552:ARG:HH21	2.17	0.57
1:A:1087:PHE:O	1:A:1091:VAL:HB	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ALA:O	1:A:609:GLN:HG3	2.04	0.57
1:A:1032:SER:O	1:A:1036:MET:HE2	2.04	0.57
1:A:222:ILE:HG13	1:A:222:ILE:O	2.03	0.57
1:A:375:ARG:HG3	1:A:376:THR:N	2.18	0.57
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.86	0.57
1:A:372:VAL:HG12	1:A:373:LEU:N	2.20	0.57
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.39	0.57
1:A:381:VAL:HG12	1:A:435:CYS:HB2	1.86	0.57
1:A:1003:SER:OG	1:A:1004:LEU:N	2.38	0.56
1:A:896:VAL:HG12	1:A:897:GLY:N	2.18	0.56
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.87	0.56
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.53	0.56
1:A:240:THR:C	1:A:242:GLY:N	2.64	0.56
1:A:682:LEU:HD22	1:A:686:LEU:HD11	1.87	0.56
1:A:239:ASP:HB3	1:A:243:THR:HB	1.88	0.56
1:A:641:ARG:HE	1:A:670:GLU:CD	2.13	0.56
1:A:965:PHE:O	1:A:966:GLY:C	2.49	0.56
1:A:1084:PHE:HE2	1:A:1088:LEU:HD11	1.69	0.56
1:A:689:LYS:HG2	1:A:728:MET:SD	2.45	0.56
1:A:741:MET:HE1	1:A:778:ASN:ND2	2.21	0.55
1:A:917:ILE:HD12	1:A:917:ILE:H	1.71	0.55
1:A:547:MET:CG	1:A:552:ARG:NH2	2.69	0.55
1:A:487:LEU:HD22	1:A:488:SER:O	2.06	0.55
1:A:1050:TYR:C	1:A:1050:TYR:CD2	2.84	0.55
1:A:1089:HIS:HA	1:A:1094:ILE:O	2.07	0.55
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.21	0.55
1:A:640:VAL:O	1:A:643:ILE:HG12	2.07	0.55
1:A:879:ILE:HD13	2:A:2095:QUE:C16	2.37	0.55
1:A:1052:ARG:HG2	1:A:1052:ARG:HH11	1.72	0.54
1:A:405:THR:CG2	1:A:407:GLU:O	2.55	0.54
1:A:731:ASP:O	1:A:735:GLN:HG3	2.07	0.54
1:A:797:VAL:HG11	1:A:800:LYS:HE3	1.90	0.54
1:A:564:LEU:HD12	1:A:1052:ARG:HB2	1.89	0.54
1:A:804:MET:HE1	1:A:831:ILE:CD1	2.38	0.54
1:A:583:LEU:HD13	1:A:610:LEU:CD2	2.38	0.54
1:A:357:CYS:HB3	1:A:420:ILE:HB	1.90	0.54
1:A:461:LEU:HD13	1:A:462:TYR:HE2	1.72	0.54
1:A:886:THR:HG22	1:A:887:THR:H	1.71	0.54
1:A:364:LYS:HE2	1:A:411:ASN:CG	2.34	0.53
1:A:1014:VAL:CG1	1:A:1065:LYS:HG3	2.31	0.53
1:A:662:GLN:HE21	1:A:1030:LEU:HD22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:CG	1:A:195:LEU:HD12	2.33	0.53
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.89	0.53
1:A:237:ALA:O	1:A:287:ILE:HG23	2.09	0.52
1:A:405:THR:HG22	1:A:408:VAL:CG2	2.39	0.52
1:A:433:ILE:HD12	1:A:484:MET:HE1	1.91	0.52
1:A:782:SER:HA	1:A:793:ALA:O	2.08	0.52
1:A:1021:ARG:C	1:A:1023:HIS:H	2.17	0.52
1:A:997:THR:HG23	1:A:1001:LYS:O	2.10	0.52
1:A:187:GLU:OE1	1:A:687:ARG:NH1	2.42	0.52
1:A:904:ASP:OD2	1:A:904:ASP:N	2.37	0.52
1:A:146:GLU:CG	1:A:319:ARG:HH12	2.23	0.52
1:A:601:GLN:NE2	1:A:602:GLU:HA	2.24	0.52
1:A:917:ILE:HD12	1:A:917:ILE:N	2.25	0.52
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.91	0.52
1:A:627:THR:HG22	1:A:644:ALA:HB1	1.90	0.52
1:A:687:ARG:HH11	1:A:687:ARG:CG	2.20	0.52
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.83	0.51
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.11	0.51
1:A:583:LEU:HD13	1:A:610:LEU:HD22	1.92	0.51
1:A:855:TRP:HB3	1:A:860:LEU:HB2	1.92	0.51
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.58	0.51
1:A:497:PHE:CB	1:A:1042:LEU:HB3	2.40	0.51
1:A:151:GLN:OE1	1:A:722:ARG:NH2	2.43	0.51
1:A:364:LYS:CE	1:A:411:ASN:OD1	2.59	0.51
1:A:929:VAL:HG22	1:A:995:MET:HE2	1.93	0.51
1:A:244:ILE:HD12	1:A:244:ILE:N	2.25	0.51
1:A:352:VAL:HG12	1:A:352:VAL:O	2.10	0.51
1:A:953:MET:HE1	2:A:2095:QUE:C2	2.41	0.51
1:A:963:ILE:O	1:A:964:ASP:C	2.52	0.50
1:A:1008:LYS:O	1:A:1012:VAL:HG23	2.11	0.50
1:A:273:ARG:NH1	1:A:308:ASP:CG	2.70	0.50
1:A:462:TYR:HB3	1:A:484:MET:HE2	1.92	0.50
1:A:945:GLY:O	1:A:985:PHE:HA	2.12	0.50
1:A:1052:ARG:HG3	1:A:1057:VAL:HG21	1.94	0.50
1:A:299:ASN:HB3	1:A:301:GLU:CG	2.29	0.50
1:A:364:LYS:HZ3	1:A:411:ASN:CG	2.15	0.50
1:A:246:GLN:O	1:A:250:THR:HG23	2.12	0.50
1:A:602:GLU:CD	1:A:602:GLU:H	2.20	0.50
1:A:782:SER:O	1:A:783:PHE:HB3	2.11	0.49
1:A:198:MET:HE3	1:A:282:VAL:HG21	1.93	0.49
1:A:874:ASP:OD1	1:A:874:ASP:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:710:GLN:HG2	1:A:711:GLN:N	2.26	0.49
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.95	0.49
1:A:509:ASP:OD2	1:A:512:ASN:HB2	2.13	0.49
1:A:531:LYS:HG3	1:A:608:TYR:CD1	2.47	0.49
1:A:900:GLY:HA2	1:A:902:PHE:CE2	2.47	0.49
1:A:396:GLN:O	1:A:397:ARG:NH1	2.46	0.49
1:A:241:PRO:HD3	1:A:285:THR:O	2.13	0.49
1:A:509:ASP:CG	1:A:512:ASN:HD22	2.20	0.49
1:A:158:ILE:HD13	1:A:717:LEU:HD13	1.95	0.49
1:A:370:ILE:HD13	1:A:514:MET:HB2	1.95	0.49
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.43	0.49
1:A:949:ASN:N	1:A:1083:GLN:HE22	2.10	0.49
1:A:169:HIS:C	1:A:169:HIS:CD2	2.90	0.48
1:A:405:THR:HG23	1:A:407:GLU:N	2.28	0.48
1:A:873:GLY:O	1:A:874:ASP:C	2.55	0.48
1:A:1021:ARG:C	1:A:1023:HIS:N	2.71	0.48
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.28	0.48
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.47	0.48
1:A:984:PRO:HG3	1:A:1071:GLN:O	2.13	0.48
1:A:239:ASP:HB3	1:A:243:THR:CB	2.43	0.48
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.13	0.48
1:A:905:GLU:H	1:A:905:GLU:CD	2.20	0.48
1:A:984:PRO:HB3	1:A:1071:GLN:OE1	2.13	0.48
1:A:220:VAL:HG22	1:A:221:PHE:N	2.28	0.48
1:A:221:PHE:N	1:A:221:PHE:CD1	2.80	0.48
1:A:635:PHE:CD1	1:A:635:PHE:N	2.82	0.48
1:A:184:ARG:NH2	1:A:321:GLU:OE1	2.46	0.48
1:A:194:LYS:O	1:A:197:ALA:N	2.47	0.48
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.49	0.48
1:A:373:LEU:HD23	1:A:406:GLU:OE2	2.14	0.48
1:A:843:LEU:HD12	1:A:843:LEU:HA	1.48	0.48
1:A:497:PHE:HB3	1:A:1042:LEU:HB3	1.96	0.48
1:A:663:LEU:HA	1:A:663:LEU:HD23	1.56	0.48
1:A:1006:PHE:CE2	1:A:1010:GLN:OE1	2.66	0.48
1:A:935:TYR:O	1:A:939:THR:HG22	2.13	0.48
1:A:955:SER:C	1:A:957:THR:N	2.68	0.48
1:A:274:VAL:HG11	1:A:292:TRP:CZ2	2.49	0.48
1:A:354:LEU:HB3	1:A:529:LEU:HD21	1.96	0.47
1:A:369:ASP:OD1	1:A:369:ASP:N	2.47	0.47
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.28	0.47
1:A:547:MET:HG3	1:A:552:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:898:ASN:O	1:A:899:THR:HG23	2.14	0.47
1:A:500:ASP:HB3	1:A:708:HIS:CD2	2.50	0.47
1:A:741:MET:O	1:A:745:VAL:HG23	2.14	0.47
1:A:784:ARG:NH1	1:A:784:ARG:HG2	2.30	0.47
1:A:929:VAL:HG22	1:A:995:MET:CE	2.44	0.47
1:A:380:THR:CG2	1:A:436:GLY:HA3	2.45	0.47
1:A:175:PHE:CE2	1:A:179:ARG:CD	2.98	0.47
1:A:405:THR:HG23	1:A:407:GLU:C	2.40	0.47
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.49	0.47
1:A:597:LYS:HD3	1:A:600:GLN:HE22	1.79	0.47
1:A:891:ILE:CG2	1:A:906:VAL:HG12	2.45	0.47
1:A:1087:PHE:HA	1:A:1091:VAL:HG23	1.96	0.47
1:A:271:VAL:CG1	1:A:310:PRO:HG3	2.45	0.47
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.36	0.47
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.45	0.47
1:A:277:ARG:NH2	1:A:788:ASP:OD2	2.33	0.47
1:A:561:THR:O	1:A:562:ASP:O	2.33	0.47
1:A:757:TYR:O	1:A:757:TYR:CD1	2.68	0.47
1:A:917:ILE:O	1:A:918:GLU:C	2.57	0.47
1:A:702:GLU:O	1:A:706:SER:HB3	2.14	0.47
1:A:760:SER:HB2	1:A:763:VAL:HB	1.97	0.47
1:A:649:GLU:HA	1:A:680:PHE:HE1	1.80	0.46
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.14	0.46
1:A:175:PHE:CZ	1:A:179:ARG:CD	2.96	0.46
1:A:271:VAL:HG22	1:A:272:LEU:N	2.30	0.46
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.15	0.46
1:A:244:ILE:HG22	1:A:245:LEU:N	2.31	0.46
1:A:273:ARG:HH11	1:A:308:ASP:CG	2.23	0.46
1:A:623:ASP:O	1:A:627:THR:OG1	2.33	0.46
1:A:876:ILE:HG22	1:A:877:GLY:N	2.30	0.46
1:A:601:GLN:HE21	1:A:602:GLU:CA	2.28	0.46
1:A:397:ARG:HD3	1:A:397:ARG:HA	1.77	0.46
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.50	0.46
1:A:841:ASP:O	1:A:845:LEU:HD22	2.15	0.46
1:A:687:ARG:O	1:A:687:ARG:HG2	2.15	0.46
1:A:380:THR:HG23	1:A:436:GLY:HA3	1.97	0.46
1:A:549:ASN:H	1:A:549:ASN:ND2	2.13	0.46
1:A:235:VAL:HG12	1:A:236:SER:N	2.31	0.45
1:A:386:ASN:OD1	1:A:396:GLN:HG3	2.16	0.45
1:A:433:ILE:CD1	1:A:484:MET:HE1	2.46	0.45
1:A:796:LEU:O	1:A:798:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.77	0.45
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.51	0.45
1:A:1045:LYS:H	1:A:1045:LYS:CD	2.20	0.45
1:A:225:HIS:CD2	1:A:823:LEU:HD11	2.51	0.45
1:A:1078:LYS:O	1:A:1079:GLY:C	2.58	0.45
1:A:163:THR:O	1:A:165:VAL:HG13	2.16	0.45
1:A:239:ASP:O	1:A:240:THR:C	2.59	0.45
1:A:932:CYS:HA	1:A:960:LEU:HD22	1.99	0.45
1:A:302:GLU:OE1	1:A:304:HIS:CE1	2.70	0.44
1:A:354:LEU:HA	1:A:529:LEU:HD21	1.99	0.44
1:A:175:PHE:CE2	1:A:179:ARG:HD3	2.53	0.44
1:A:196:TYR:OH	1:A:728:MET:CE	2.65	0.44
1:A:876:ILE:HG22	1:A:877:GLY:H	1.82	0.44
1:A:955:SER:O	1:A:957:THR:N	2.50	0.44
1:A:181:VAL:O	1:A:185:MET:HG2	2.18	0.44
1:A:192:ASP:OD2	1:A:194:LYS:N	2.50	0.44
1:A:842:MET:O	1:A:843:LEU:C	2.59	0.44
1:A:896:VAL:HG12	1:A:897:GLY:H	1.83	0.44
1:A:980:LYS:HB2	1:A:981:GLU:H	1.69	0.44
1:A:405:THR:HG23	1:A:407:GLU:O	2.18	0.44
1:A:1087:PHE:O	1:A:1087:PHE:CD1	2.71	0.44
1:A:162:VAL:HG13	1:A:714:ALA:HB1	1.99	0.44
1:A:302:GLU:OE1	1:A:304:HIS:HE1	2.00	0.44
1:A:632:ASP:HB3	1:A:1033:MET:HE3	2.00	0.44
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.53	0.44
1:A:192:ASP:OD2	1:A:192:ASP:C	2.61	0.43
1:A:914:LYS:HD2	1:A:956:GLU:CD	2.43	0.43
1:A:1031:PHE:CG	1:A:1051:ILE:HD13	2.53	0.43
1:A:270:PHE:O	1:A:271:VAL:HB	2.19	0.43
1:A:1010:GLN:HG2	1:A:1069:LEU:HD21	1.99	0.43
1:A:1087:PHE:CD1	1:A:1087:PHE:C	2.96	0.43
1:A:738:VAL:HG12	1:A:742:LEU:HD12	2.00	0.43
1:A:554:GLN:NE2	1:A:554:GLN:HA	2.33	0.43
1:A:199:HIS:O	1:A:200:PRO:C	2.61	0.43
1:A:547:MET:CE	1:A:552:ARG:HA	2.41	0.43
1:A:552:ARG:HE	1:A:552:ARG:HB2	1.48	0.43
1:A:768:LYS:O	1:A:772:GLU:CG	2.66	0.43
1:A:147:THR:HA	1:A:319:ARG:NH2	2.33	0.43
1:A:211:LEU:CD2	1:A:298:LYS:HB2	2.42	0.43
1:A:303:ILE:CG2	1:A:305:LEU:HD21	2.44	0.43
1:A:759:VAL:O	1:A:760:SER:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:THR:HG22	1:A:887:THR:N	2.34	0.43
1:A:1031:PHE:HB2	1:A:1051:ILE:HD13	2.01	0.43
1:A:243:THR:C	1:A:244:ILE:O	2.55	0.43
1:A:529:LEU:N	1:A:529:LEU:HD23	2.34	0.43
1:A:917:ILE:H	1:A:917:ILE:CD1	2.32	0.43
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.01	0.42
1:A:682:LEU:HD22	1:A:686:LEU:HD12	2.01	0.42
1:A:362:ARG:NH2	1:A:413:TRP:CH2	2.87	0.42
1:A:611:LEU:HD13	1:A:639:ASN:ND2	2.35	0.42
1:A:927:ARG:O	1:A:928:PHE:C	2.62	0.42
1:A:960:LEU:HG	1:A:961:PHE:N	2.34	0.42
1:A:487:LEU:CD2	1:A:488:SER:N	2.80	0.42
1:A:862:LEU:HD13	1:A:862:LEU:HA	1.81	0.42
1:A:983:VAL:HG22	1:A:984:PRO:CD	2.36	0.42
1:A:233:ILE:HG22	1:A:234:LYS:O	2.18	0.42
1:A:353:SER:C	1:A:354:LEU:HG	2.43	0.42
1:A:564:LEU:CD1	1:A:1052:ARG:HB2	2.48	0.42
1:A:798:ILE:HD12	1:A:798:ILE:N	2.30	0.42
1:A:200:PRO:HG3	1:A:282:VAL:HG23	2.00	0.42
1:A:1028:ILE:HD13	1:A:1051:ILE:HG23	2.00	0.42
1:A:370:ILE:O	1:A:370:ILE:CG2	2.67	0.42
1:A:576:TRP:O	1:A:579:ARG:CG	2.53	0.42
1:A:815:PHE:O	1:A:827:THR:HB	2.19	0.42
1:A:380:THR:HA	1:A:402:LYS:O	2.20	0.42
1:A:406:GLU:H	1:A:406:GLU:HG2	1.56	0.42
1:A:380:THR:O	1:A:435:CYS:HA	2.20	0.42
1:A:462:TYR:CB	1:A:484:MET:HE2	2.49	0.42
1:A:624:VAL:O	1:A:628:MET:HG2	2.20	0.42
1:A:776:ASN:O	1:A:777:LEU:HD12	2.19	0.42
1:A:208:PRO:HG3	1:A:856:GLU:HG2	2.02	0.41
1:A:295:GLN:O	1:A:299:ASN:HB2	2.20	0.41
1:A:364:LYS:NZ	1:A:411:ASN:CG	2.77	0.41
1:A:611:LEU:O	1:A:612:ALA:C	2.63	0.41
1:A:352:VAL:HA	1:A:527:ILE:HD11	2.01	0.41
1:A:472:ARG:HB2	1:A:474:LEU:HG	2.03	0.41
1:A:907:LEU:HD22	1:A:994:VAL:CG2	2.46	0.41
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	2.02	0.41
1:A:296:CYS:O	1:A:297:LEU:C	2.61	0.41
1:A:523:TYR:HD2	1:A:526:PRO:HG3	1.85	0.41
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.49	0.41
1:A:181:VAL:O	1:A:185:MET:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLN:CA	1:A:554:GLN:HE21	2.34	0.41
1:A:1010:GLN:HG2	1:A:1069:LEU:CD2	2.50	0.41
1:A:470:ASP:OD1	1:A:472:ARG:N	2.45	0.41
1:A:952:ILE:HD13	1:A:962:HIS:CD2	2.56	0.41
1:A:1062:GLU:O	1:A:1063:ASP:C	2.63	0.41
1:A:373:LEU:HD12	1:A:374:PRO:N	2.36	0.41
1:A:514:MET:HB2	1:A:514:MET:HE2	2.00	0.41
1:A:590:PRO:HG3	1:A:630:LEU:HD21	2.03	0.41
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.21	0.41
1:A:921:PHE:CD2	1:A:921:PHE:C	2.99	0.41
1:A:1066:LYS:O	1:A:1067:TYR:C	2.63	0.41
1:A:653:ASP:OD2	1:A:688:ASN:ND2	2.53	0.41
1:A:705:GLN:NE2	1:A:839:ARG:NE	2.69	0.41
1:A:948:HIS:CG	1:A:949:ASN:N	2.88	0.41
1:A:995:MET:HE1	1:A:1009:PHE:HB2	2.03	0.41
1:A:154:LEU:O	1:A:155:ASN:C	2.64	0.40
1:A:363:VAL:HG23	1:A:520:LEU:CD1	2.50	0.40
1:A:389:TYR:O	1:A:392:GLN:HB3	2.21	0.40
1:A:477:HIS:HA	1:A:520:LEU:HB3	2.04	0.40
1:A:1089:HIS:CD2	1:A:1089:HIS:C	2.99	0.40
1:A:309:THR:HA	1:A:310:PRO:HD3	1.91	0.40
1:A:371:PRO:C	1:A:372:VAL:HG23	2.47	0.40
1:A:380:THR:O	1:A:436:GLY:N	2.45	0.40
1:A:187:GLU:CD	1:A:687:ARG:NH1	2.79	0.40
1:A:244:ILE:HG22	1:A:245:LEU:H	1.86	0.40
1:A:561:THR:O	1:A:562:ASP:C	2.64	0.40
1:A:964:ASP:HA	2:A:2095:QUE:O24	2.20	0.40
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.97	0.40
1:A:648:LEU:C	1:A:650:SER:N	2.80	0.40
1:A:760:SER:O	1:A:763:VAL:N	2.54	0.40
1:A:903:LYS:HB2	1:A:906:VAL:HG23	2.04	0.40
1:A:768:LYS:O	1:A:772:GLU:HG3	2.22	0.40
1:A:1059:LYS:HA	1:A:1059:LYS:HD3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	837/961 (87%)	738 (88%)	84 (10%)	15 (2%)	6	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	ALA
1	A	524	CYS
1	A	753	SER
1	A	776	ASN
1	A	874	ASP
1	A	896	VAL
1	A	783	PHE
1	A	356	ASP
1	A	956	GLU
1	A	217	ASN
1	A	271	VAL
1	A	980	LYS
1	A	1022	HIS
1	A	562	ASP
1	A	1079	GLY

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	767/857 (90%)	666 (87%)	101 (13%)	4	8

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	154	LEU
1	A	162	VAL
1	A	172	GLU
1	A	185	MET
1	A	192	ASP
1	A	203	THR
1	A	212	LEU
1	A	227	SER
1	A	231	GLN
1	A	238	ASP
1	A	251	LYS
1	A	252	MET
1	A	282	VAL
1	A	287	ILE
1	A	305	LEU
1	A	320	LYS
1	A	354	LEU
1	A	355	TRP
1	A	356	ASP
1	A	357	CYS
1	A	362	ARG
1	A	366	ARG
1	A	369	ASP
1	A	373	LEU
1	A	388	GLN
1	A	393	VAL
1	A	406	GLU
1	A	418	ILE
1	A	435	CYS
1	A	461	LEU
1	A	467	LEU
1	A	487	LEU
1	A	516	ILE
1	A	520	LEU
1	A	521	ASP
1	A	527	ILE
1	A	529	LEU
1	A	532	HIS
1	A	546	GLU
1	A	550	GLN
1	A	551	LEU

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Mol	Chain	Res	Type
1	A	552	ARG
1	A	554	GLN
1	A	561	THR
1	A	574	LEU
1	A	575	LEU
1	A	601	GLN
1	A	603	ILE
1	A	610	LEU
1	A	626	LEU
1	A	627	THR
1	A	662	GLN
1	A	682	LEU
1	A	687	ARG
1	A	710	GLN
1	A	717	LEU
1	A	729	LEU
1	A	737	GLN
1	A	750	LYS
1	A	755	GLU
1	A	766	GLN
1	A	792	LYS
1	A	816	LYS
1	A	823	LEU
1	A	841	ASP
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	865	LEU
1	A	874	ASP
1	A	876	ILE
1	A	887	THR
1	A	890	LYS
1	A	899	THR
1	A	904	ASP
1	A	905	GLU
1	A	913	GLU
1	A	919	GLU
1	A	927	ARG
1	A	947	ARG
1	A	949	ASN
1	A	952	ILE
1	A	954	ILE

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Mol	Chain	Res	Type
1	A	957	THR
1	A	960	LEU
1	A	1010	GLN
1	A	1026	LEU
1	A	1027	LEU
1	A	1029	ILE
1	A	1036	MET
1	A	1039	MET
1	A	1041	GLN
1	A	1046	GLU
1	A	1051	ILE
1	A	1059	LYS
1	A	1063	ASP
1	A	1075	CYS
1	A	1076	ARG
1	A	1082	VAL
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	HIS
1	A	218	ASN
1	A	225	HIS
1	A	291	GLN
1	A	295	GLN
1	A	304	HIS
1	A	459	GLN
1	A	522	ASN
1	A	549	ASN
1	A	554	GLN
1	A	601	GLN
1	A	634	ASN
1	A	639	ASN
1	A	662	GLN
1	A	705	GLN
1	A	708	HIS
1	A	737	GLN
1	A	769	GLN
1	A	825	ASN
1	A	951	ASN

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Mol	Chain	Res	Type
1	A	959	ASN
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	QUE	A	2095	-	24,24,24	4.38	14 (58%)	36,36,36	3.23	19 (52%)

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	QUE	A	2095	-	-	0/4/4/4	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	QUE	C10-C11	14.46	1.50	1.36
2	A	2095	QUE	C1-C2	7.51	1.49	1.38
2	A	2095	QUE	C1-C6	5.55	1.47	1.39
2	A	2095	QUE	C19-C14	5.08	1.47	1.39
2	A	2095	QUE	C16-C15	4.63	1.46	1.38
2	A	2095	QUE	C15-C14	4.63	1.46	1.39
2	A	2095	QUE	O12-C11	3.75	1.42	1.37
2	A	2095	QUE	C5-C4	3.38	1.44	1.38
2	A	2095	QUE	C19-C18	3.38	1.43	1.38
2	A	2095	QUE	C16-C17	3.21	1.45	1.39
2	A	2095	QUE	C18-C17	3.10	1.45	1.40
2	A	2095	QUE	O24-C17	2.93	1.42	1.36
2	A	2095	QUE	O29-C6	2.59	1.42	1.37
2	A	2095	QUE	C3-C2	2.07	1.44	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	QUE	C11-C10-C9	-9.56	114.69	121.52
2	A	2095	QUE	C14-C19-C18	6.59	125.84	120.09
2	A	2095	QUE	O27-C10-C11	6.14	127.09	120.74
2	A	2095	QUE	C2-C3-C4	-5.12	112.52	117.41
2	A	2095	QUE	C5-C6-C1	-4.81	113.88	120.47
2	A	2095	QUE	C15-C14-C11	4.34	127.10	120.71
2	A	2095	QUE	O12-C4-C3	-4.20	117.07	121.19
2	A	2095	QUE	C2-C3-C9	3.79	127.05	121.45
2	A	2095	QUE	C3-C9-C10	3.72	122.15	116.88
2	A	2095	QUE	C19-C18-C17	-3.37	116.77	119.89
2	A	2095	QUE	C4-O12-C11	3.33	125.78	120.67
2	A	2095	QUE	C15-C14-C19	-3.32	115.41	119.25
2	A	2095	QUE	O29-C6-C1	2.85	127.32	119.85
2	A	2095	QUE	C2-C1-C6	2.67	122.14	119.67
2	A	2095	QUE	C5-C4-C3	2.55	126.22	121.79
2	A	2095	QUE	O13-C9-C10	-2.44	114.66	119.61
2	A	2095	QUE	C4-C5-C6	2.38	122.73	118.98
2	A	2095	QUE	C19-C14-C11	-2.25	117.48	120.65
2	A	2095	QUE	O12-C11-C14	2.24	114.00	110.87

There are no chirality outliers.

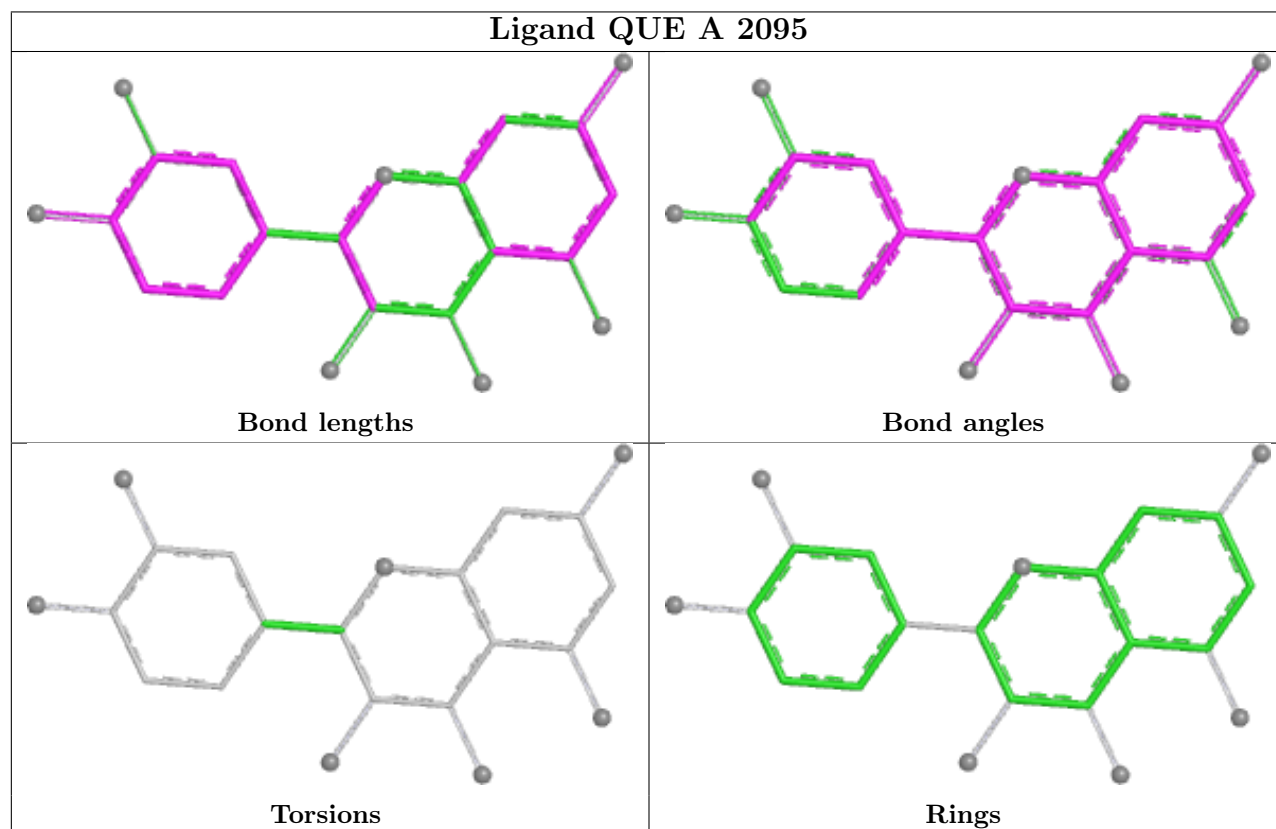
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2095	QUE	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	851/961 (88%)	0.61	67 (7%) 18 16	25, 65, 104, 119	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	874	ASP	4.1
1	A	352	VAL	3.6
1	A	917	ILE	3.4
1	A	527	ILE	3.2
1	A	991	PHE	3.2
1	A	529	LEU	3.2
1	A	895	THR	3.0
1	A	374	PRO	2.9
1	A	409	LEU	2.9
1	A	752	LEU	2.9
1	A	249	PHE	2.9
1	A	987	LEU	2.8
1	A	764	ILE	2.8
1	A	481	VAL	2.8
1	A	757	TYR	2.8
1	A	759	VAL	2.8
1	A	168	VAL	2.7
1	A	896	VAL	2.7
1	A	528	ALA	2.7
1	A	211	LEU	2.7
1	A	252	MET	2.7
1	A	1004	LEU	2.6
1	A	767	LEU	2.6
1	A	907	LEU	2.5
1	A	924	ALA	2.5
1	A	1040	PRO	2.5
1	A	519	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	996	GLY	2.5
1	A	921	PHE	2.5
1	A	215	ILE	2.4
1	A	233	ILE	2.4
1	A	235	VAL	2.4
1	A	994	VAL	2.4
1	A	901	ALA	2.4
1	A	754	ALA	2.4
1	A	520	LEU	2.3
1	A	358	ASP	2.3
1	A	354	LEU	2.3
1	A	763	VAL	2.3
1	A	532	HIS	2.2
1	A	373	LEU	2.2
1	A	919	GLU	2.2
1	A	1084	PHE	2.2
1	A	297	LEU	2.2
1	A	992	LEU	2.2
1	A	521	ASP	2.2
1	A	1082	VAL	2.2
1	A	1094	ILE	2.2
1	A	404	PHE	2.2
1	A	1064	ALA	2.1
1	A	555	LEU	2.1
1	A	558	ILE	2.1
1	A	886	THR	2.1
1	A	244	ILE	2.1
1	A	313	PRO	2.1
1	A	413	TRP	2.1
1	A	376	THR	2.1
1	A	250	THR	2.1
1	A	990	ASP	2.1
1	A	993	PHE	2.0
1	A	1009	PHE	2.0
1	A	771	LEU	2.0
1	A	777	LEU	2.0
1	A	1090	LEU	2.0
1	A	222	ILE	2.0
1	A	948	HIS	2.0
1	A	272	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](#)

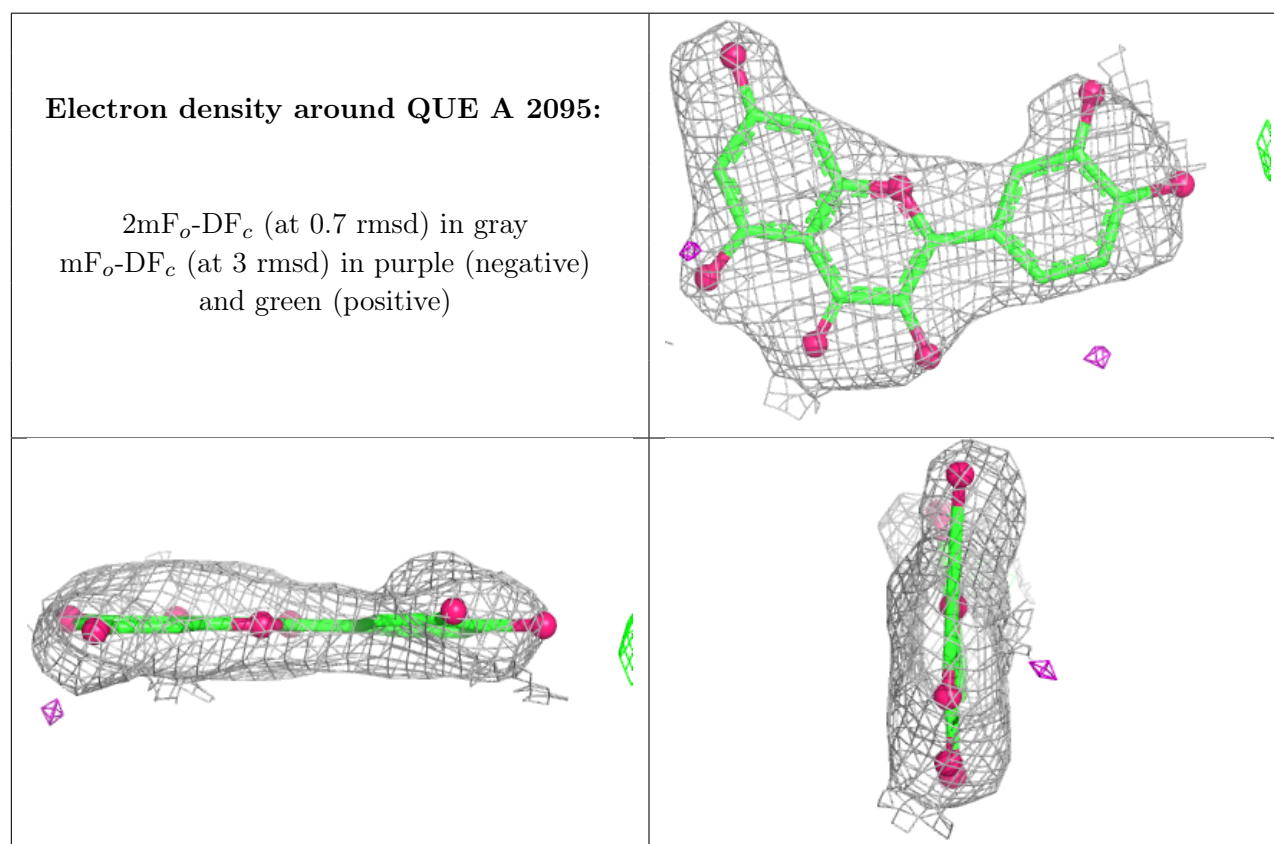
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	QUE	A	2095	22/22	0.88	0.12	69,73,75,75	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.