Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 10:59 am GMT

PDB ID	:	1E8W
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)

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

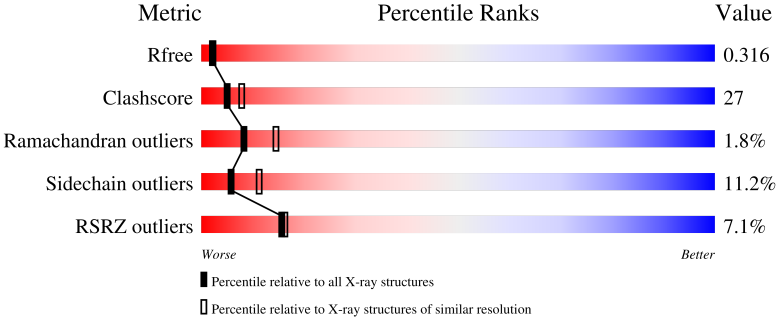
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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.

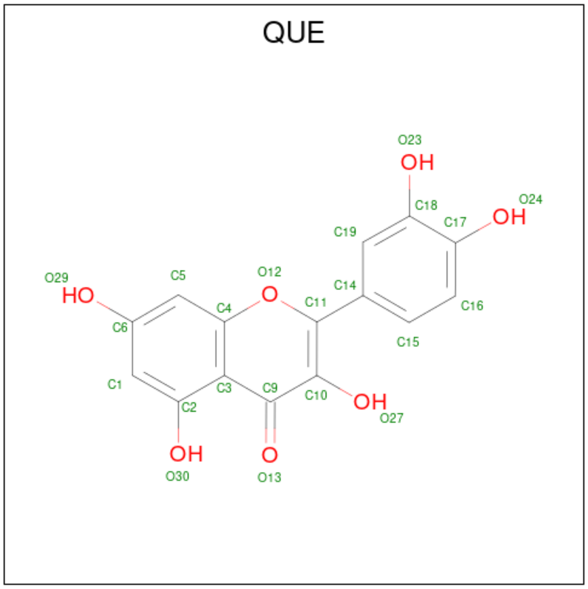
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE CATALYTIC SUBUNIT.

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 (three-letter code: QUE) (formula: $C_{15}H_{10}O_7$).



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

SEQUENCE-PLOTS INFOmissingINFO

3 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
$< I/\sigma(I) >$ [1]	2.39 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.265 , 0.330 0.248 , 0.316	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 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	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.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 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	0.93	6/7039 (0.1%)	0.94	9/9524 (0.1%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	915	CYS	CB-SG	-8.13	1.68	1.82
1	A	787	TYR	CD2-CE2	6.49	1.49	1.39
1	A	697	TRP	CZ3-CH2	5.85	1.49	1.40
1	A	867	TYR	CE2-CZ	-5.31	1.31	1.38
1	A	668	LYS	CD-CE	5.17	1.64	1.51
1	A	842	MET	SD-CE	-5.10	1.49	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	837	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	A	632	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	357	CYS	N-CA-C	-5.85	95.22	111.00
1	A	674	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	653	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	690	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	191	ARG	NE-CZ-NH2	5.21	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	847	ILE	CG1-CB-CG2	-5.08	100.23	111.40
1	A	837	ASP	CB-CG-OD2	5.03	122.83	118.30

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

4.2 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	377	0
2	A	22	0	10	2	0
All	All	6915	0	6973	377	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 (377) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:410:TRP:HB3	1:A:412:VAL:HG23	1.72	0.70
1:A:418:ILE:HG13	1:A:419:LYS:N	2.07	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

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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:180:LEU:C	1:A:183:PRO:HD2	2.16	0.66
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: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
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:629:GLN:HG2	1:A:1029:ILE:HG13	1.79	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:601:GLN:HE21	1:A:602:GLU:HA	1.65	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:1032:SER:O	1:A:1036:MET:HE2	2.00	0.61
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.15	0.61
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:N	1:A:233:ILE:HD12	2.16	0.61
1:A:150:PHE:HD1	1:A:153:GLN:NE2	1.99	0.61
1:A:181:VAL:HG12	1:A:185:MET:CE	2.31	0.61
1:A:743:GLN:O	1:A:747:ILE:HD12	2.01	0.60
1:A:955:SER:C	1:A:957:THR:H	2.04	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:855:TRP:CE3	1:A:862:LEU:HD23	2.37	0.59
1:A:689:LYS:HG2	1:A:728:MET:HE2	1.82	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: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:232:THR:C	1:A:233:ILE:HD12	2.24	0.58
1:A:240:THR:C	1:A:242:GLY:H	2.07	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
1:A:605:ALA:O	1:A:609:GLN:HG3	2.04	0.57
1:A:222:ILE:HG13	1:A:222:ILE:O	2.03	0.57
1:A:498:ASN:OD1	1:A:498:ASN:C	2.41	0.57
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.86	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:1064:ALA:O	1:A:1065:LYS:C	2.43	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:181:VAL:HG12	1:A:185:MET:HE2	1.87	0.56
1:A:225:HIS:HE1	1:A:304:HIS:HD2	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:PHE:HE2	1:A:1088:LEU:HD11	1.69	0.56
1:A:561:THR:HG21	1:A:565:ASN:CG	2.27	0.56
1:A:689:LYS:HG2	1:A:728:MET:SD	2.45	0.56
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: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:547:MET:HE1	1:A:552:ARG:HA	1.89	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: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
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:782:SER:HA	1:A:793:ALA:O	2.08	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:240:THR:C	1:A:242:GLY:N	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:PHE:O	1:A:966:GLY:C	2.49	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:547:MET:CE	1:A:552:ARG:HA	2.41	0.51
1:A:886:THR:C	1:A:953:MET:HE2	2.31	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:641:ARG:HE	1:A:670:GLU:CD	2.13	0.50
1:A:1008:LYS:O	1:A:1012:VAL:HG23	2.11	0.50
1:A:1050:TYR:C	1:A:1050:TYR:CD2	2.84	0.50
1:A:782:SER:O	1:A:783:PHE:HB3	2.11	0.50
1:A:874:ASP:OD1	1:A:874:ASP:N	2.41	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:246:GLN:O	1:A:250:THR:HG23	2.12	0.50
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:842:MET:HE3	1:A:870:ILE:HD13	1.91	0.49
1:A:241:PRO:HD3	1:A:285:THR:O	2.13	0.49
1:A:158:ILE:HD13	1:A:717:LEU:HD13	1.95	0.49
1:A:192:ASP:CG	1:A:195:LEU:HD12	2.33	0.49
1:A:364:LYS:HE2	1:A:411:ASN:CG	2.34	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:405:THR:HG23	1:A:407:GLU:N	2.28	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: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

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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:1021:ARG:C	1:A:1023:HIS:H	2.17	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
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:842:MET:HE2	1:A:870:ILE:HD13	1.97	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: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: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:623:ASP:O	1:A:627:THR:OG1	2.33	0.46

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
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:462:TYR:HB2	1:A:484:MET:HE1	1.98	0.46
1:A:841:ASP:O	1:A:845:LEU:HD22	2.15	0.46
1:A:273:ARG:NH1	1:A:308:ASP:CG	2.70	0.46
1:A:687:ARG:O	1:A:687:ARG:HG2	2.15	0.46
1:A:741:MET:HE3	1:A:778:ASN:ND2	2.31	0.46
1:A:963:ILE:O	1:A:964:ASP:C	2.52	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:796:LEU:O	1:A:798:ILE:HD12	2.16	0.45
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:602:GLU:CD	1:A:602:GLU:H	2.20	0.45
1:A:929:VAL:HG22	1:A:995:MET:HE3	1.98	0.45
1:A:163:THR:O	1:A:165:VAL:HG13	2.16	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:955:SER:C	1:A:957:THR:N	2.68	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:HG12	1:A:185:MET:HE1	1.99	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:509:ASP:CG	1:A:512:ASN:HD22	2.20	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:1021:ARG:C	1:A:1023:HIS:N	2.71	0.44
1:A:405:THR:HG23	1:A:407:GLU:O	2.18	0.44
1:A:873:GLY:O	1:A:874:ASP:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:C	1:A:169:HIS:CD2	2.90	0.44
1:A:302:GLU:OE1	1:A:304:HIS:HE1	2.00	0.44
1:A:586:PRO:HA	1:A:589:TYR:CE1	2.53	0.44
1:A:554:GLN:HA	1:A:554:GLN:NE2	2.33	0.43
1:A:905:GLU:H	1:A:905:GLU:CD	2.20	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:738:VAL:HG12	1:A:742:LEU:HD12	2.00	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:886:THR:HG22	1:A:887:THR:N	2.34	0.43
1:A:462:TYR:CB	1:A:484:MET:HE1	2.49	0.43
1:A:1031:PHE:HB2	1:A:1051:ILE:HD13	2.01	0.43
1:A:433:ILE:HD12	1:A:484:MET:HE1	2.01	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:405:THR:HG23	1:A:407:GLU:C	2.40	0.42
1:A:611:LEU:HD13	1:A:639:ASN:ND2	2.35	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: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:917:ILE:O	1:A:918:GLU:C	2.57	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:948:HIS:CG	1:A:949:ASN:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:THR:O	1:A:435:CYS:HA	2.20	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:243:THR:C	1:A:244:ILE:O	2.55	0.41
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:273:ARG:HH11	1:A:308:ASP:CG	2.23	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: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
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:373:LEU:HD12	1:A:374:PRO:N	2.36	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:741:MET:HE2	1:A:774:LEU:HD22	2.03	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: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:309:THR:HA	1:A:310:PRO:HD3	1.91	0.40
1:A:380:THR:O	1:A:436:GLY:N	2.45	0.40
1:A:244:ILE:HG22	1:A:245:LEU:H	1.86	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: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:833:LYS:NZ	1:A:836:ASP:OD2	2.50	0.40
1:A:1059:LYS:HA	1:A:1059:LYS:HD3	1.83	0.40
1:A:1078:LYS:O	1:A:1079:GLY:C	2.58	0.40

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 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%)	8 14

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

4.3.2 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%)	681 (89%)	86 (11%)	6 11

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
1	A	172	GLU
1	A	185	MET
1	A	192	ASP
1	A	203	THR
1	A	225	HIS
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	299	ASN
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	369	ASP
1	A	373	LEU
1	A	388	GLN
1	A	393	VAL
1	A	404	PHE
1	A	406	GLU
1	A	410	TRP
1	A	418	ILE
1	A	435	CYS
1	A	461	LEU
1	A	487	LEU
1	A	516	ILE
1	A	521	ASP
1	A	529	LEU
1	A	532	HIS
1	A	546	GLU
1	A	550	GLN
1	A	551	LEU
1	A	552	ARG
1	A	554	GLN
1	A	561	THR
1	A	574	LEU

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Mol	Chain	Res	Type
1	A	575	LEU
1	A	601	GLN
1	A	610	LEU
1	A	626	LEU
1	A	682	LEU
1	A	687	ARG
1	A	710	GLN
1	A	717	LEU
1	A	737	GLN
1	A	766	GLN
1	A	775	GLN
1	A	776	ASN
1	A	807	LYS
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	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
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	1039	MET
1	A	1041	GLN
1	A	1045	LYS
1	A	1046	GLU
1	A	1051	ILE
1	A	1059	LYS
1	A	1063	ASP

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Mol	Chain	Res	Type
1	A	1075	CYS
1	A	1076	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	169	HIS
1	A	291	GLN
1	A	304	HIS
1	A	396	GLN
1	A	459	GLN
1	A	522	ASN
1	A	549	ASN
1	A	554	GLN
1	A	600	GLN
1	A	601	GLN
1	A	639	ASN
1	A	662	GLN
1	A	705	GLN
1	A	743	GLN
1	A	778	ASN
1	A	825	ASN
1	A	951	ASN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN
1	A	1089	HIS

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

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	-	21,24,24	3.10	12 (57%)	27,36,36	3.01	12 (44%)

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	-	-	0/0/4/4	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2095	QUE	C19-C18	6.44	1.43	1.37
2	A	2095	QUE	C1-C6	5.57	1.47	1.39
2	A	2095	QUE	C1-C2	5.26	1.49	1.37
2	A	2095	QUE	C15-C16	4.60	1.46	1.36
2	A	2095	QUE	C5-C4	3.49	1.44	1.37
2	A	2095	QUE	O12-C11	3.37	1.42	1.36
2	A	2095	QUE	C18-C17	3.22	1.45	1.40
2	A	2095	QUE	C16-C17	3.14	1.45	1.39
2	A	2095	QUE	O24-C17	2.86	1.42	1.36
2	A	2095	QUE	O29-C6	2.48	1.42	1.37
2	A	2095	QUE	C5-C6	2.43	1.41	1.37
2	A	2095	QUE	C19-C14	2.24	1.47	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2095	QUE	C5-C6-C1	-8.75	113.88	120.94
2	A	2095	QUE	C18-C19-C14	5.68	125.84	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2095	QUE	C19-C18-C17	-5.10	116.77	119.86
2	A	2095	QUE	C2-C3-C4	-4.57	112.52	117.82
2	A	2095	QUE	O27-C10-C11	4.07	127.09	119.62
2	A	2095	QUE	O12-C4-C3	-4.02	117.07	121.03
2	A	2095	QUE	C2-C3-C9	3.03	127.05	121.85
2	A	2095	QUE	O29-C6-C1	2.88	127.32	119.84
2	A	2095	QUE	C5-C4-C3	2.87	126.22	123.05
2	A	2095	QUE	C2-C1-C6	2.70	122.14	119.70
2	A	2095	QUE	C19-C14-C15	-2.20	115.41	118.15
2	A	2095	QUE	C11-C10-C9	-2.14	114.69	118.75

There are no chirality outliers.

There are no torsion outliers.

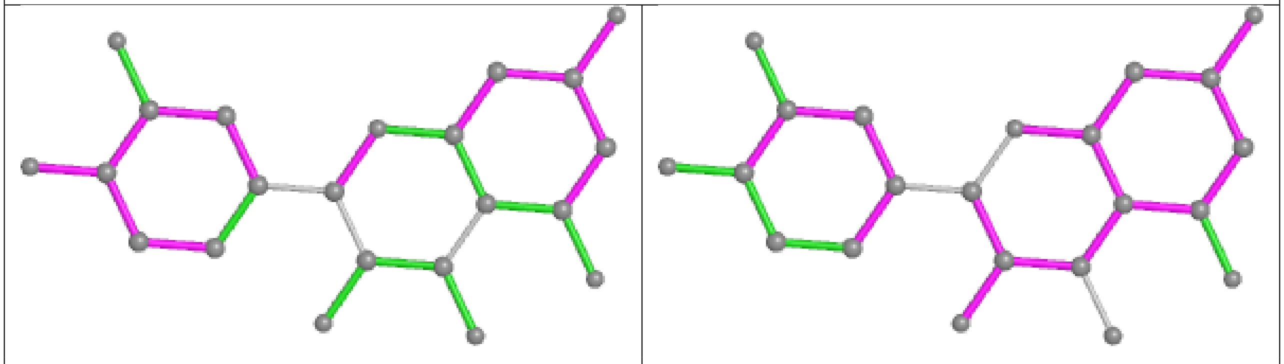
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2095	QUE	2	0

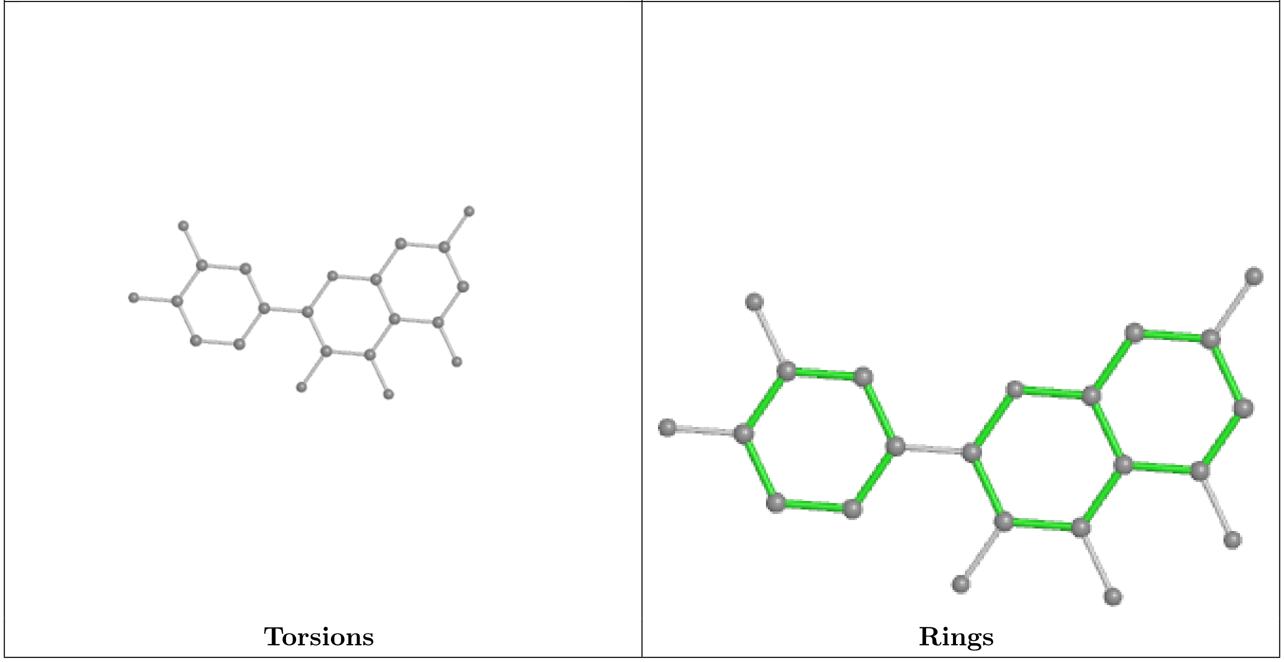
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand QUE A 2095



Bond lengths

Bond angles



Torsions

Rings

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 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, 95^{th} 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%)	0.45	60 (7%)	16	16	25, 65, 104, 119	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1040	PRO	5.7
1	A	529	LEU	5.5
1	A	211	LEU	5.3
1	A	374	PRO	4.8
1	A	558	ILE	4.8
1	A	907	LEU	4.5
1	A	998	SER	4.3
1	A	991	PHE	4.3
1	A	895	THR	4.0
1	A	375	ARG	4.0
1	A	353	SER	3.6
1	A	823	LEU	3.5
1	A	527	ILE	3.5
1	A	248	PHE	3.4
1	A	245	LEU	3.4
1	A	919	GLU	3.3
1	A	1048	ILE	3.3
1	A	896	VAL	3.3
1	A	987	LEU	3.2
1	A	270	PHE	3.2
1	A	992	LEU	3.2
1	A	307	LEU	3.1
1	A	994	VAL	3.1
1	A	523	TYR	3.0
1	A	874	ASP	3.0
1	A	917	ILE	3.0
1	A	222	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1057	VAL	2.8
1	A	475	LEU	2.8
1	A	224	ILE	2.8
1	A	409	LEU	2.7
1	A	359	ARG	2.7
1	A	365	ILE	2.7
1	A	993	PHE	2.6
1	A	924	ALA	2.6
1	A	771	LEU	2.6
1	A	310	PRO	2.5
1	A	481	VAL	2.5
1	A	707	ARG	2.5
1	A	466	LEU	2.5
1	A	525	HIS	2.4
1	A	282	VAL	2.4
1	A	358	ASP	2.4
1	A	767	LEU	2.4
1	A	524	CYS	2.4
1	A	252	MET	2.3
1	A	920	LYS	2.3
1	A	996	GLY	2.3
1	A	410	TRP	2.3
1	A	404	PHE	2.3
1	A	143	ALA	2.3
1	A	379	LEU	2.2
1	A	413	TRP	2.2
1	A	429	LEU	2.2
1	A	898	ASN	2.2
1	A	168	VAL	2.1
1	A	754	ALA	2.1
1	A	761	SER	2.1
1	A	930	TYR	2.1
1	A	272	LEU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

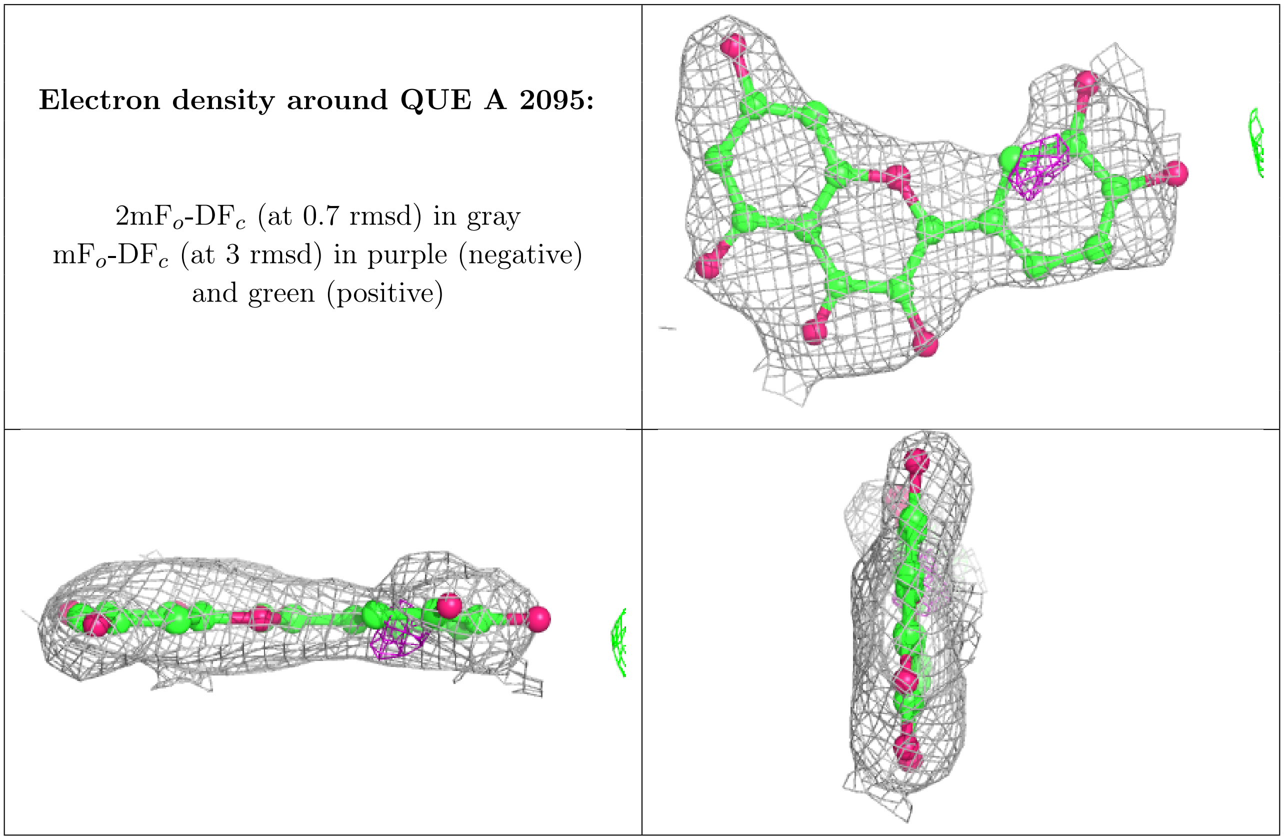
There are no monosaccharides in this entry.

5.4 Ligands

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
2	QUE	A	2095	22/22	0.86	0.28	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.



Electron density around QUE A 2095:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

5.5 Other polymers

There are no such residues in this entry.