



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:27 AM UTC

PDB ID : 3PS6 / pdb_00003ps6
Title : Quinazolines with intra-molecular hydrogen bonding scaffold (iMHBS) as PI3K/mTOR dual inhibitors.
Authors : Knighton, D.R.; Greasley, S.E.; Rogers, C.M.-L.
Deposited on : 2010-11-30
Resolution : 2.60 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

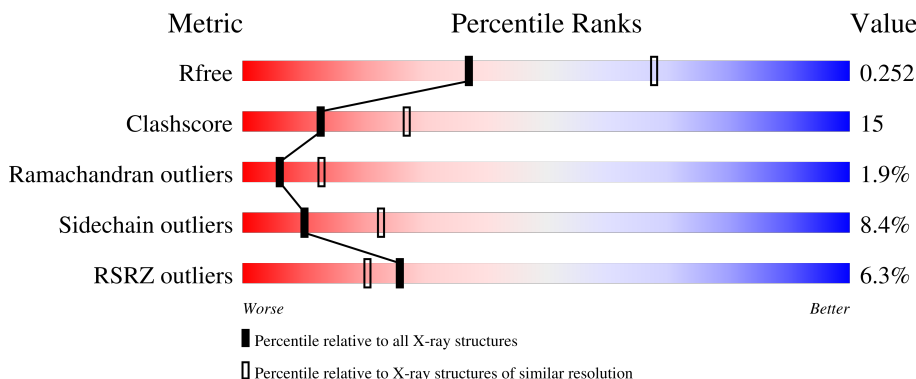
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 6802 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.

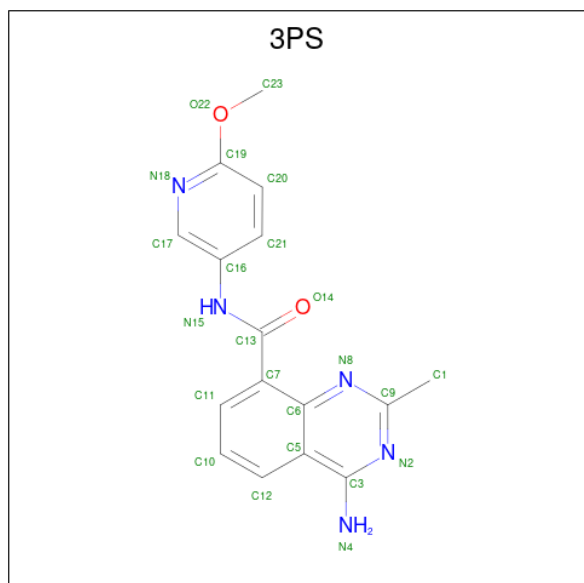
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	841	Total	C	N	O	S	0	0	0
			6779	4364	1147	1233	35			

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 4-amino-N-(6-methoxypyridin-3-yl)-2-methylquinazoline-8-carboxamide (CCD ID: 3PS) (formula: C₁₆H₁₅N₅O₂).

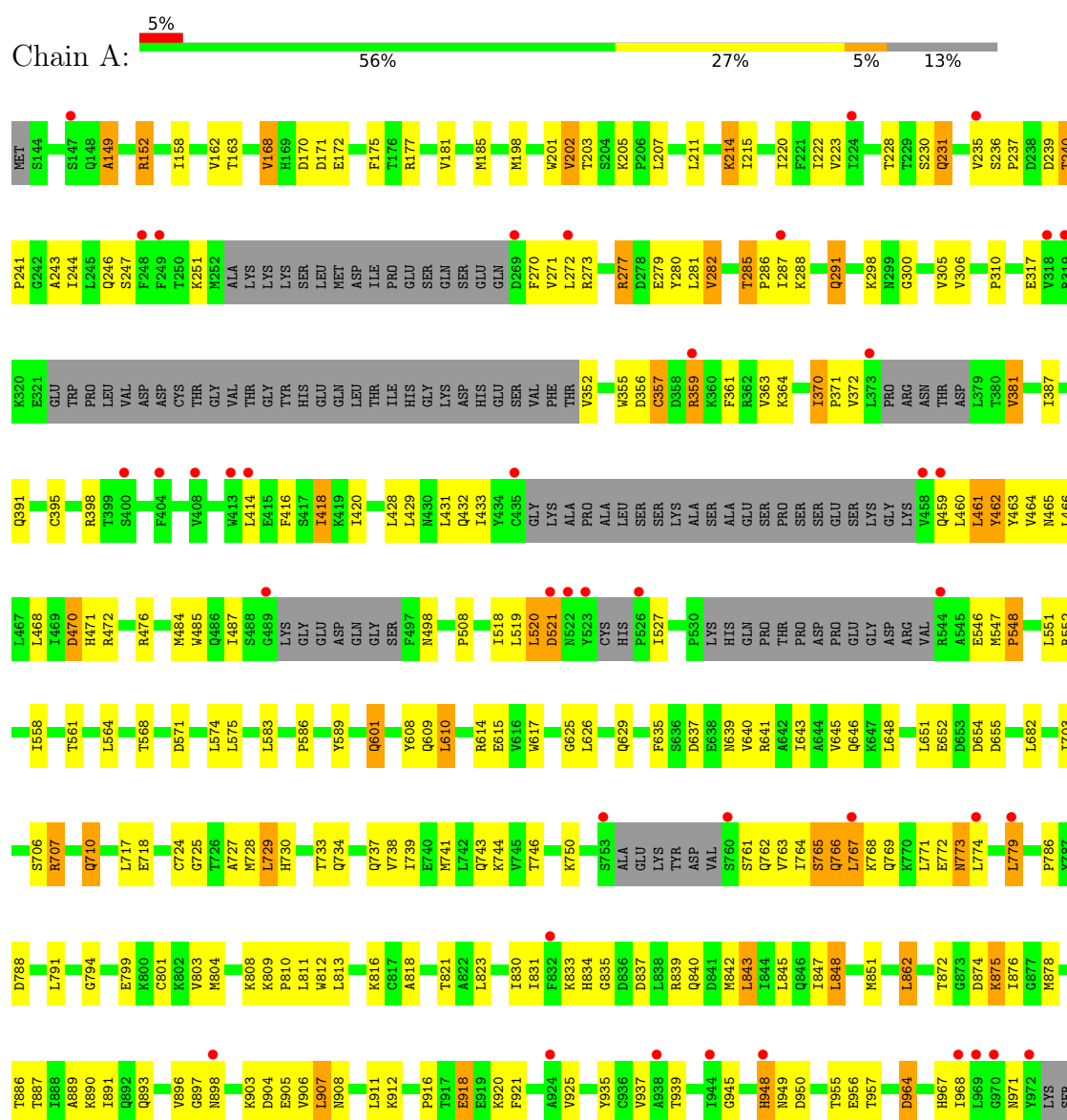


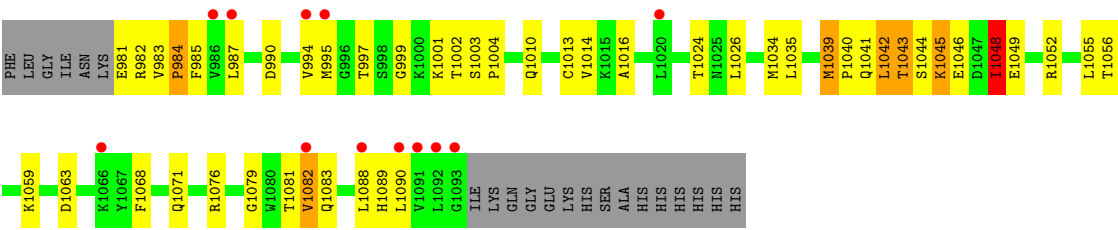
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			23	16	5	2		

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	144.04Å 67.49Å 106.64Å 90.00° 95.50° 90.00°	Depositor
Resolution (Å)	44.76 – 2.60 44.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.76-2.60) 97.9 (44.76-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	CNS, BUSTER 2.9.6	Depositor
R, R_{free}	0.256 , 0.251 0.260 , 0.252	Depositor DCC
R_{free} test set	1557 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6802	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: 3PS

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	0.80	7/6924 (0.1%)	1.41	29/9371 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	462	TYR	CA-C	-11.85	1.37	1.52
1	A	356	ASP	CA-C	-9.54	1.40	1.52
1	A	356	ASP	C-O	-6.26	1.15	1.24
1	A	520	LEU	C-O	-5.88	1.17	1.24
1	A	1089	HIS	CA-CB	5.74	1.60	1.53
1	A	1089	HIS	CB-CG	5.15	1.57	1.50
1	A	461	LEU	CB-CG	-5.06	1.43	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	ASP	CA-C-N	-10.72	107.41	123.07
1	A	356	ASP	C-N-CA	-10.72	107.41	123.07
1	A	357	CYS	N-CA-CB	9.34	125.40	110.65
1	A	1088	LEU	CA-C-N	8.62	133.69	121.71
1	A	1088	LEU	C-N-CA	8.62	133.69	121.71
1	A	637	ASP	CA-C-N	6.71	129.59	120.54
1	A	637	ASP	C-N-CA	6.71	129.59	120.54
1	A	918	GLU	N-CA-C	-6.66	105.31	113.50
1	A	498	ASN	CA-C-N	6.17	128.83	120.38
1	A	498	ASN	C-N-CA	6.17	128.83	120.38
1	A	1056	THR	CB-CA-C	5.75	121.08	112.06
1	A	246	GLN	N-CA-C	-5.64	106.26	113.02
1	A	470	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	470	ASP	CA-C-N	5.57	129.51	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	ASP	C-N-CA	5.57	129.51	120.60
1	A	381	VAL	N-CA-C	5.53	115.65	108.35
1	A	773	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	765	SER	CA-C-N	5.37	127.79	120.54
1	A	765	SER	C-N-CA	5.37	127.79	120.54
1	A	149	ALA	CA-C-N	5.21	127.21	120.44
1	A	149	ALA	C-N-CA	5.21	127.21	120.44
1	A	1063	ASP	CA-C-N	5.14	127.43	120.65
1	A	1063	ASP	C-N-CA	5.14	127.43	120.65
1	A	937	VAL	CA-C-N	5.11	127.38	120.38
1	A	937	VAL	C-N-CA	5.11	127.38	120.38
1	A	609	GLN	CA-C-N	5.08	127.51	120.29
1	A	609	GLN	C-N-CA	5.08	127.51	120.29
1	A	1048	ILE	CA-C-N	5.07	127.78	120.38
1	A	1048	ILE	C-N-CA	5.07	127.78	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6779	0	6801	204	0
2	A	23	0	15	3	0
All	All	6802	0	6816	205	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 15.

All (205) 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:202:VAL:HG11	1:A:285:THR:HG21	1.37	1.04
1:A:887:THR:HB	1:A:890:LYS:HD2	1.46	0.98
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:THR:HG21	1:A:1076:ARG:HH12	1.44	0.82
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.66	0.77
1:A:558:ILE:O	1:A:561:THR:HG22	1.85	0.77
1:A:202:VAL:CG1	1:A:285:THR:HG21	2.17	0.74
1:A:903:LYS:HE2	1:A:905:GLU:HB3	1.70	0.74
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.68	0.74
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.69	0.72
1:A:997:THR:CG2	1:A:1076:ARG:HH12	2.04	0.70
1:A:903:LYS:HB3	1:A:906:VAL:HG23	1.74	0.70
1:A:746:THR:HA	1:A:811:LEU:HD11	1.71	0.70
1:A:162:VAL:HG21	1:A:718:GLU:OE1	1.92	0.69
1:A:804:MET:HE2	1:A:812:TRP:HB2	1.73	0.69
1:A:764:ILE:O	1:A:768:LYS:HG2	1.92	0.69
1:A:547:MET:HB3	1:A:552:ARG:HH12	1.55	0.69
1:A:215:ILE:HD11	1:A:220:ILE:HD11	1.75	0.68
1:A:235:VAL:HG13	1:A:239:ASP:HB2	1.77	0.66
1:A:181:VAL:HG12	1:A:185:MET:HE2	1.77	0.66
1:A:847:ILE:HG22	1:A:851:MET:HE2	1.76	0.66
1:A:908:ASN:HD22	1:A:994:VAL:HA	1.59	0.66
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.78	0.65
1:A:149:ALA:HA	1:A:152:ARG:NH1	2.11	0.65
1:A:835:GLY:H	1:A:875:LYS:HB3	1.61	0.65
1:A:568:THR:HG23	1:A:571:ASP:H	1.62	0.65
1:A:964:ASP:HA	2:A:1:3PS:H23A	1.80	0.64
1:A:240:THR:HG23	1:A:243:ALA:HB3	1.79	0.64
1:A:291:GLN:HE21	1:A:291:GLN:HA	1.61	0.64
1:A:1035:LEU:HD12	1:A:1048:ILE:HD13	1.81	0.62
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.14	0.62
1:A:470:ASP:HB3	1:A:476:ARG:HH21	1.64	0.62
1:A:983:VAL:HG12	1:A:1082:VAL:HG11	1.82	0.62
1:A:1001:LYS:HG2	1:A:1002:THR:H	1.65	0.62
1:A:564:LEU:HB2	1:A:1052:ARG:HD2	1.82	0.62
1:A:241:PRO:HD3	1:A:285:THR:O	2.00	0.61
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.36	0.61
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.83	0.61
1:A:984:PRO:HB2	1:A:985:PHE:CD2	2.36	0.60
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.66	0.59
1:A:152:ARG:HH11	1:A:152:ARG:HB2	1.66	0.59
1:A:461:LEU:HB3	1:A:462:TYR:CE2	2.37	0.59
1:A:359:ARG:HB2	1:A:359:ARG:HH11	1.68	0.59
1:A:202:VAL:HG12	1:A:203:THR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:PRO:HG3	1:A:707:ARG:HD3	1.85	0.58
1:A:948:HIS:N	1:A:948:HIS:CD2	2.71	0.58
1:A:546:GLU:HG3	1:A:547:MET:H	1.68	0.58
1:A:935:TYR:O	1:A:939:THR:HG22	2.04	0.58
1:A:359:ARG:O	1:A:420:ILE:HG12	2.04	0.58
1:A:741:MET:HE1	1:A:779:LEU:HA	1.85	0.58
1:A:921:PHE:O	1:A:925:VAL:HG23	2.03	0.58
1:A:271:VAL:HG23	1:A:282:VAL:HG13	1.87	0.57
1:A:734:GLN:O	1:A:738:VAL:HG23	2.04	0.57
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	2.19	0.56
1:A:804:MET:HE1	1:A:831:ILE:HG12	1.87	0.56
1:A:987:LEU:HD11	1:A:995:MET:HE1	1.86	0.56
1:A:520:LEU:O	1:A:521:ASP:C	2.49	0.55
2:A:1:3PS:N8	2:A:1:3PS:N15	2.45	0.55
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.87	0.55
1:A:725:GLY:O	1:A:729:LEU:HB2	2.07	0.55
1:A:767:LEU:HD12	1:A:803:VAL:HG23	1.88	0.55
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.88	0.55
1:A:706:SER:O	1:A:710:GLN:HB3	2.06	0.55
1:A:767:LEU:O	1:A:771:LEU:HG	2.06	0.55
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.88	0.55
1:A:222:ILE:HD12	1:A:235:VAL:HG21	1.88	0.55
1:A:786:PRO:HD2	1:A:878:MET:HE1	1.89	0.55
1:A:761:SER:HA	1:A:764:ILE:HD12	1.89	0.54
1:A:955:THR:C	1:A:957:THR:H	2.16	0.54
1:A:352:VAL:O	1:A:527:ILE:HA	2.08	0.54
1:A:387:ILE:HD12	1:A:418:ILE:HD12	1.89	0.54
1:A:431:LEU:O	1:A:463:TYR:HA	2.08	0.54
1:A:625:GLY:O	1:A:629:GLN:HG3	2.07	0.54
1:A:464:VAL:HB	1:A:484:MET:HG2	1.90	0.53
1:A:843:LEU:HG	1:A:1034:MET:HG3	1.90	0.53
1:A:803:VAL:CG1	1:A:809:LYS:HB3	2.40	0.52
1:A:908:ASN:ND2	1:A:994:VAL:HA	2.24	0.52
1:A:763:VAL:HA	1:A:766:GLN:HE22	1.74	0.52
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.92	0.52
1:A:948:HIS:CD2	1:A:948:HIS:H	2.26	0.52
1:A:767:LEU:HD22	1:A:771:LEU:HD11	1.91	0.51
1:A:848:LEU:HD12	1:A:851:MET:CE	2.40	0.51
1:A:239:ASP:O	1:A:287:ILE:HG13	2.10	0.51
1:A:461:LEU:HB3	1:A:462:TYR:CD2	2.45	0.51
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.26	0.51
1:A:398:ARG:O	1:A:414:LEU:HD21	2.11	0.50
1:A:750:LYS:HE3	1:A:834:HIS:O	2.11	0.50
1:A:801:CYS:HA	1:A:812:TRP:O	2.11	0.50
1:A:198:MET:HB3	1:A:282:VAL:HG21	1.94	0.50
1:A:171:ASP:CG	1:A:472:ARG:HH12	2.19	0.50
1:A:839:ARG:HA	1:A:842:MET:HE2	1.94	0.50
1:A:466:LEU:CD1	1:A:476:ARG:HH11	2.25	0.49
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.77	0.49
1:A:945:GLY:C	1:A:985:PHE:HA	2.38	0.49
1:A:766:GLN:H	1:A:766:GLN:NE2	2.10	0.49
1:A:903:LYS:HB3	1:A:906:VAL:CG2	2.43	0.49
1:A:273:ARG:O	1:A:305:VAL:HG13	2.13	0.48
1:A:739:ILE:O	1:A:743:GLN:HG3	2.14	0.48
1:A:285:THR:HG22	1:A:286:PRO:HD2	1.96	0.48
1:A:774:LEU:O	1:A:779:LEU:HB3	2.14	0.48
1:A:743:GLN:NE2	1:A:872:THR:OG1	2.47	0.48
1:A:236:SER:HB3	1:A:239:ASP:OD1	2.14	0.47
1:A:462:TYR:CB	1:A:484:MET:HE2	2.44	0.47
1:A:466:LEU:HD11	1:A:476:ARG:HH11	1.79	0.47
1:A:874:ASP:C	1:A:876:ILE:H	2.22	0.47
1:A:270:PHE:HA	1:A:310:PRO:HD3	1.96	0.47
1:A:361:PHE:CD2	1:A:387:ILE:HD11	2.49	0.47
1:A:1083:GLN:NE2	1:A:1083:GLN:HA	2.29	0.47
1:A:198:MET:CB	1:A:282:VAL:HG21	2.44	0.47
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.97	0.47
1:A:762:GLN:O	1:A:766:GLN:NE2	2.49	0.46
1:A:908:ASN:HA	1:A:911:LEU:HD12	1.97	0.46
1:A:983:VAL:HG23	1:A:984:PRO:HD2	1.97	0.46
1:A:240:THR:HG23	1:A:243:ALA:CB	2.45	0.46
1:A:746:THR:HA	1:A:811:LEU:CD1	2.41	0.46
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.16	0.46
1:A:168:VAL:HG13	1:A:170:ASP:H	1.81	0.46
1:A:635:PHE:O	1:A:641:ARG:HD2	2.16	0.46
1:A:983:VAL:CG1	1:A:1082:VAL:HG11	2.45	0.46
1:A:171:ASP:O	1:A:175:PHE:HB2	2.16	0.46
1:A:277:ARG:NH2	1:A:788:ASP:OD2	2.46	0.46
1:A:277:ARG:NH2	1:A:791:LEU:HG	2.30	0.46
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.98	0.46
1:A:207:LEU:HB2	1:A:288:LYS:HD2	1.97	0.46
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:THR:HA	1:A:1055:LEU:HD13	1.98	0.46
1:A:552:ARG:HH11	1:A:552:ARG:HB2	1.81	0.46
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.96	0.46
1:A:803:VAL:HG13	1:A:809:LYS:HB3	1.98	0.46
1:A:370:ILE:HD12	1:A:372:VAL:O	2.16	0.45
1:A:280:TYR:HB3	1:A:282:VAL:HG22	1.97	0.45
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.17	0.45
1:A:247:SER:C	1:A:251:LYS:HB2	2.42	0.45
1:A:149:ALA:HA	1:A:152:ARG:HH11	1.78	0.45
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.32	0.45
1:A:862:LEU:HD11	1:A:1016:ALA:HB2	1.98	0.45
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.47	0.45
1:A:903:LYS:HG2	1:A:905:GLU:H	1.83	0.44
1:A:1040:PRO:C	1:A:1042:LEU:H	2.25	0.44
1:A:887:THR:HG22	1:A:889:ALA:H	1.83	0.44
1:A:462:TYR:HA	1:A:485:TRP:O	2.17	0.44
1:A:733:THR:HG22	1:A:737:GLN:NE2	2.33	0.44
1:A:810:PRO:HB3	1:A:833:LYS:HB2	1.99	0.44
1:A:463:TYR:CD2	1:A:487:ILE:HD11	2.52	0.44
1:A:520:LEU:O	1:A:521:ASP:O	2.35	0.44
1:A:741:MET:HB3	1:A:774:LEU:HD13	1.99	0.44
1:A:887:THR:CG2	1:A:950:ASP:HA	2.47	0.44
1:A:948:HIS:HE1	1:A:967:HIS:HD2	1.65	0.44
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.48	0.44
1:A:462:TYR:HB3	1:A:484:MET:HE2	1.98	0.44
1:A:990:ASP:O	1:A:994:VAL:HG23	2.18	0.44
1:A:306:VAL:HG21	1:A:821:THR:CG2	2.48	0.44
1:A:985:PHE:CD2	1:A:985:PHE:N	2.86	0.44
1:A:395:CYS:HB2	1:A:418:ILE:HD11	2.00	0.43
1:A:230:SER:O	1:A:231:GLN:HB2	2.18	0.43
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.43
1:A:763:VAL:HA	1:A:766:GLN:NE2	2.33	0.43
1:A:997:THR:HG21	1:A:1076:ARG:NH1	2.23	0.43
1:A:558:ILE:HG21	1:A:575:LEU:CD2	2.35	0.43
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.99	0.43
1:A:608:TYR:CE1	1:A:639:ASN:ND2	2.87	0.43
1:A:640:VAL:O	1:A:643:ILE:HG12	2.19	0.43
1:A:277:ARG:HH22	1:A:788:ASP:CG	2.26	0.42
1:A:786:PRO:HD2	1:A:878:MET:CE	2.47	0.42
1:A:355:TRP:NE1	1:A:601:GLN:HE22	2.17	0.42
1:A:794:GLY:CA	1:A:818:ALA:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:O	1:A:244:ILE:HG13	2.19	0.42
1:A:652:GLU:HG3	1:A:654:ASP:HB3	2.02	0.42
1:A:984:PRO:HG2	1:A:1071:GLN:O	2.20	0.42
1:A:840:GLN:HA	1:A:1039:MET:HE1	2.00	0.42
1:A:158:ILE:HG23	1:A:703:ILE:HD13	2.01	0.42
1:A:761:SER:HA	1:A:764:ILE:CD1	2.50	0.42
1:A:912:LYS:NZ	1:A:918:GLU:HG2	2.35	0.42
1:A:558:ILE:CG2	1:A:575:LEU:HD21	2.36	0.42
1:A:765:SER:O	1:A:769:GLN:HG3	2.20	0.42
1:A:907:LEU:HD23	1:A:911:LEU:HD11	2.00	0.42
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.85	0.42
1:A:364:LYS:O	1:A:518:ILE:HA	2.19	0.42
1:A:548:PRO:HD2	1:A:551:LEU:HD12	2.02	0.42
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.55	0.42
1:A:848:LEU:HD12	1:A:851:MET:HE3	2.02	0.41
1:A:918:GLU:O	1:A:921:PHE:HB3	2.20	0.41
1:A:768:LYS:O	1:A:772:GLU:HG3	2.21	0.41
1:A:830:ILE:HG21	1:A:878:MET:HE3	2.03	0.41
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.56	0.41
1:A:995:MET:O	1:A:1003:SER:OG	2.38	0.41
1:A:1045:LYS:HE3	1:A:1049:GLU:OE1	2.21	0.41
1:A:152:ARG:NH1	1:A:152:ARG:HB2	2.32	0.41
1:A:162:VAL:HG23	1:A:163:THR:N	2.36	0.41
1:A:547:MET:O	1:A:548:PRO:O	2.38	0.41
1:A:811:LEU:HD23	1:A:813:LEU:HD21	2.03	0.41
1:A:830:ILE:CG2	1:A:878:MET:HB2	2.51	0.41
1:A:964:ASP:OD1	2:A:1:3PS:H23B	2.20	0.41
1:A:1001:LYS:O	1:A:1076:ARG:NH2	2.46	0.40
1:A:1043:THR:O	1:A:1045:LYS:N	2.55	0.40
1:A:1035:LEU:CD2	1:A:1039:MET:HG3	2.45	0.40
1:A:163:THR:HG22	1:A:177:ARG:HH12	1.85	0.40
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.57	0.40
1:A:211:LEU:HD21	1:A:298:LYS:HA	2.03	0.40
1:A:241:PRO:HB3	1:A:281:LEU:O	2.22	0.40
1:A:433:ILE:HG13	1:A:484:MET:HE1	2.02	0.40
1:A:891:ILE:O	1:A:906:VAL:HG11	2.22	0.40
1:A:981:GLU:C	1:A:982:ARG:HG3	2.46	0.40
1:A:750:LYS:NZ	1:A:834:HIS:HD2	2.18	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	821/966 (85%)	727 (89%)	78 (10%)	16 (2%)	6	13

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	548	PRO
1	A	971	ASN
1	A	1044	SER
1	A	1045	LYS
1	A	896	VAL
1	A	897	GLY
1	A	999	GLY
1	A	1079	GLY
1	A	521	ASP
1	A	956	GLU
1	A	228	THR
1	A	237	PRO
1	A	875	LYS
1	A	371	PRO
1	A	984	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	748/864 (87%)	685 (92%)	63 (8%)	10 23

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	ARG
1	A	168	VAL
1	A	202	VAL
1	A	205	LYS
1	A	214	LYS
1	A	223	VAL
1	A	240	THR
1	A	277	ARG
1	A	279	GLU
1	A	282	VAL
1	A	285	THR
1	A	291	GLN
1	A	317	GLU
1	A	357	CYS
1	A	359	ARG
1	A	370	ILE
1	A	381	VAL
1	A	391	GLN
1	A	418	ILE
1	A	459	GLN
1	A	574	LEU
1	A	601	GLN
1	A	610	LEU
1	A	615	GLU
1	A	626	LEU
1	A	646	GLN
1	A	682	LEU
1	A	707	ARG
1	A	710	GLN
1	A	717	LEU
1	A	729	LEU
1	A	744	LYS
1	A	766	GLN
1	A	767	LEU
1	A	773	ASN

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Mol	Chain	Res	Type
1	A	779	LEU
1	A	799	GLU
1	A	808	LYS
1	A	816	LYS
1	A	823	LEU
1	A	843	LEU
1	A	845	LEU
1	A	848	LEU
1	A	862	LEU
1	A	886	THR
1	A	893	GLN
1	A	898	ASN
1	A	904	ASP
1	A	907	LEU
1	A	948	HIS
1	A	964	ASP
1	A	968	ILE
1	A	1026	LEU
1	A	1039	MET
1	A	1041	GLN
1	A	1042	LEU
1	A	1043	THR
1	A	1046	GLU
1	A	1048	ILE
1	A	1059	LYS
1	A	1081	THR
1	A	1082	VAL
1	A	1090	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	217	ASN
1	A	291	GLN
1	A	304	HIS
1	A	391	GLN
1	A	396	GLN
1	A	554	GLN
1	A	600	GLN
1	A	601	GLN
1	A	734	GLN

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Mol	Chain	Res	Type
1	A	737	GLN
1	A	743	GLN
1	A	762	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	834	HIS
1	A	840	GLN
1	A	893	GLN
1	A	898	ASN
1	A	908	ASN
1	A	909	HIS
1	A	922	GLN
1	A	951	ASN
1	A	959	ASN
1	A	967	HIS
1	A	1007	GLN
1	A	1083	GLN
1	A	1085	ASN

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	3PS	A	1	-	25,25,25	2.34	8 (32%)	32,35,35	2.06	10 (31%)

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	3PS	A	1	-	-	6/10/10/10	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	3PS	C3-C5	-6.91	1.38	1.45
2	A	1	3PS	C17-C16	5.01	1.48	1.39
2	A	1	3PS	C7-C6	-3.16	1.38	1.43
2	A	1	3PS	C21-C16	-2.92	1.34	1.39
2	A	1	3PS	C21-C20	2.84	1.43	1.38
2	A	1	3PS	C20-C19	-2.66	1.34	1.39
2	A	1	3PS	C17-N18	2.45	1.39	1.34
2	A	1	3PS	C12-C5	-2.05	1.38	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	3PS	C16-C17-N18	-5.66	119.39	124.07
2	A	1	3PS	C17-N18-C19	4.52	120.83	116.72
2	A	1	3PS	C20-C21-C16	4.39	125.35	120.30
2	A	1	3PS	C21-C16-C17	-3.80	114.09	117.78
2	A	1	3PS	O14-C13-C7	-2.89	118.02	121.73
2	A	1	3PS	O22-C19-C20	-2.75	111.90	116.77
2	A	1	3PS	C9-N2-C3	-2.23	114.66	118.10
2	A	1	3PS	C1-C9-N8	-2.07	114.04	117.13
2	A	1	3PS	N8-C9-N2	2.07	129.39	125.77
2	A	1	3PS	O22-C19-N18	2.03	123.39	119.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

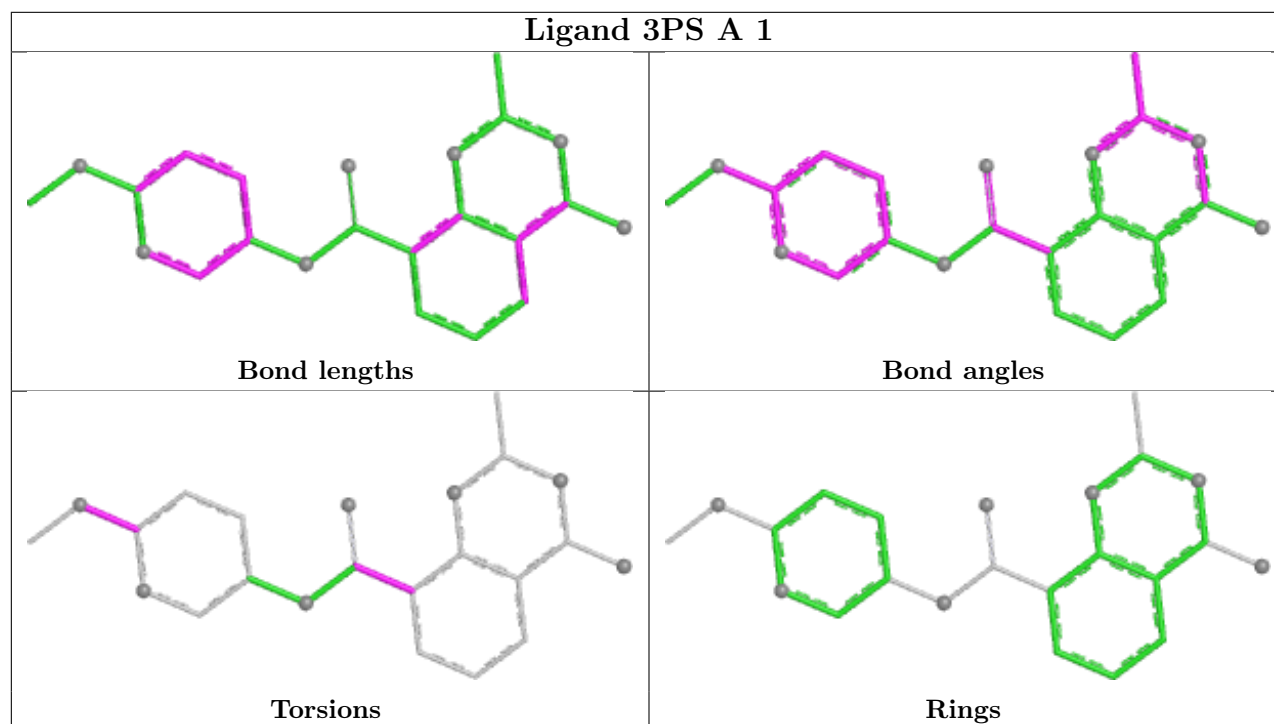
Mol	Chain	Res	Type	Atoms
2	A	1	3PS	N18-C19-O22-C23
2	A	1	3PS	C20-C19-O22-C23
2	A	1	3PS	O14-C13-C7-C11
2	A	1	3PS	O14-C13-C7-C6
2	A	1	3PS	N15-C13-C7-C11
2	A	1	3PS	N15-C13-C7-C6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	3PS	3	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	841/966 (87%)	0.68	53 (6%)	26 20	33, 74, 112, 140	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	TYR	4.6
1	A	235	VAL	3.4
1	A	767	LEU	3.3
1	A	318	VAL	3.3
1	A	938	ALA	3.2
1	A	319	ARG	3.2
1	A	522	ASN	3.1
1	A	359	ARG	2.9
1	A	249	PHE	2.9
1	A	1090	LEU	2.9
1	A	972	TYR	2.8
1	A	987	LEU	2.8
1	A	1093	GLY	2.8
1	A	373	LEU	2.8
1	A	969	LEU	2.8
1	A	1082	VAL	2.7
1	A	521	ASP	2.7
1	A	753	SER	2.6
1	A	1091	VAL	2.6
1	A	489	GLY	2.6
1	A	272	LEU	2.6
1	A	526	PRO	2.6
1	A	898	ASN	2.5
1	A	970	GLY	2.5
1	A	760	SER	2.4
1	A	459	GLN	2.4
1	A	1088	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1092	LEU	2.3
1	A	1066	LYS	2.3
1	A	774	LEU	2.3
1	A	248	PHE	2.3
1	A	986	VAL	2.2
1	A	147	SER	2.2
1	A	779	LEU	2.2
1	A	994	VAL	2.2
1	A	995	MET	2.2
1	A	413	TRP	2.2
1	A	968	ILE	2.2
1	A	400	SER	2.2
1	A	544	ARG	2.1
1	A	269	ASP	2.1
1	A	408	VAL	2.1
1	A	944	ILE	2.1
1	A	832	PHE	2.1
1	A	435	CYS	2.1
1	A	948	HIS	2.1
1	A	224	ILE	2.1
1	A	1020	LEU	2.1
1	A	404	PHE	2.1
1	A	924	ALA	2.0
1	A	287	ILE	2.0
1	A	414	LEU	2.0
1	A	458	VAL	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](#)

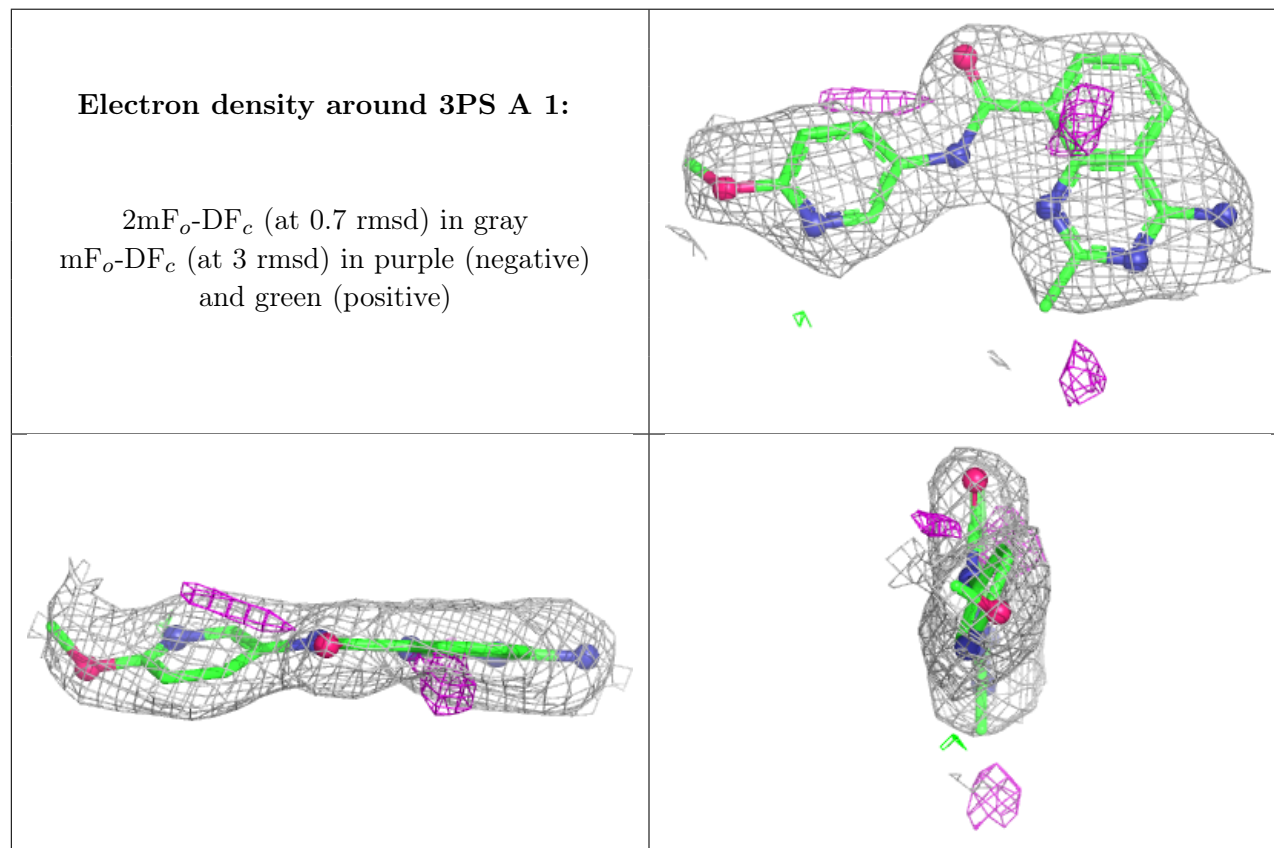
There are no oligosaccharides in this entry.

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	3PS	A	1	23/23	0.86	0.12	58,61,65,66	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.