



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:11 AM GMT

PDB ID : 3L54
Title : Structure of Pi3K gamma with inhibitor
Authors : Elkins, P.A.; Smallwood, A.M.
Deposited on : 2009-12-21
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

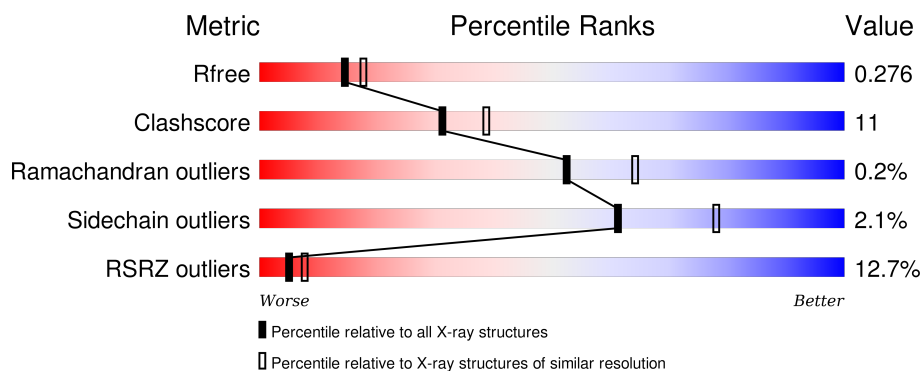
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>11%</div> <div>65%</div> <div>21%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6836 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	837	Total	C	N	O	S	3	0	0
			6779	4363	1153	1228	35			

There are 11 discrepancies between the modelled and reference sequences:

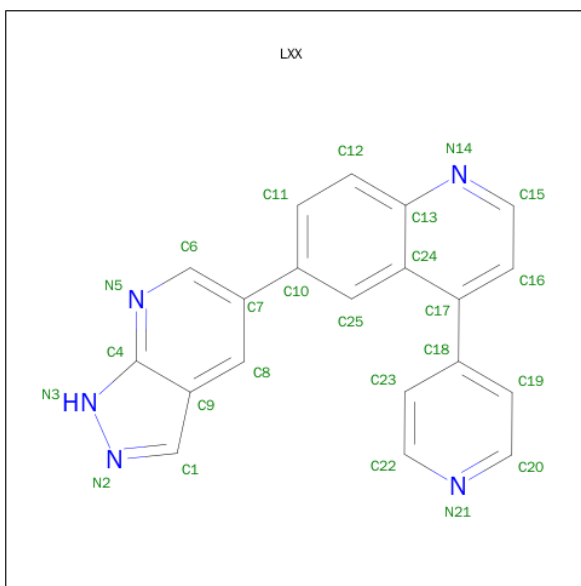
Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736
A	295	GLN	HIS	CONFLICT	UNP P48736
A	777	LEU	SER	CONFLICT	UNP P48736
A	778	ASN	GLN	CONFLICT	UNP P48736
A	1012	VAL	ILE	CONFLICT	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP 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 SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 6-(1H-PYRAZOLO[3,4-B]PYRIDIN-5-YL)-4-PYRIDIN-4-YLQUINOLINE (three-letter code: LXX) (formula: C₂₀H₁₃N₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			25	20	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total	O	0	0
			27	27		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.26 Å 68.41 Å 106.72 Å 90.00° 94.76° 90.00°	Depositor
Resolution (Å)	39.43 – 2.30 41.05 – 2.30	Depositor EDS
% Data completeness (in resolution range)	81.1 (39.43-2.30) 81.1 (41.05-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 2.29 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.216 , 0.280 0.218 , 0.276	Depositor DCC
R_{free} test set	1895 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 37798 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6836	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, LXX

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	0.27	0/6923	0.43	0/9368

There are no bond length outliers.

There are no bond angle outliers.

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	6833	146	0
2	A	5	0	0	0	0
3	A	25	0	13	1	0
4	A	27	0	0	0	0
All	All	6836	0	6846	147	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 11.

All (147) 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:798:ILE:H	1:A:798:ILE:HD12	1.35	0.91
1:A:1041:GLN:HG2	1:A:1042:LEU:HD13	1.50	0.89
1:A:955:THR:HG22	1:A:957:THR:H	1.39	0.86
1:A:896:VAL:HG11	1:A:901:ALA:HB3	1.60	0.83
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.63	0.80
1:A:181:VAL:O	1:A:185:MET:HG3	1.85	0.76
1:A:355:TRP:HA	1:A:421:LYS:HB2	1.67	0.75
1:A:887:THR:HG22	1:A:889:ALA:H	1.51	0.75
1:A:775:GLN:OE1	1:A:798:ILE:HD11	1.91	0.71
1:A:739:ILE:HG23	1:A:832:PHE:HZ	1.56	0.71
1:A:935:TYR:O	1:A:939:THR:HB	1.93	0.69
1:A:219:CYS:SG	1:A:234:LYS:HG3	2.33	0.68
1:A:693:HIS:CD2	1:A:789:PRO:HG3	2.29	0.68
1:A:738:VAL:HA	1:A:741:MET:HE2	1.77	0.67
1:A:947:ARG:HD3	1:A:968:ILE:HD12	1.78	0.66
1:A:498:ASN:ND2	1:A:1040:PRO:HB3	2.10	0.65
1:A:424:PRO:HG3	1:A:598:TRP:O	1.96	0.65
1:A:917:THR:OG1	1:A:919:GLU:HG2	1.95	0.65
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.80	0.63
1:A:800:LYS:CB	1:A:814:GLU:HG3	2.30	0.61
1:A:1092:LEU:HD12	1:A:1093:GLY:N	2.15	0.61
1:A:1092:LEU:HD11	1:A:1094:ILE:HG13	1.83	0.60
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.83	0.60
1:A:625:GLY:O	1:A:629:GLN:HG3	2.02	0.60
1:A:798:ILE:CD1	1:A:798:ILE:H	2.12	0.60
1:A:887:THR:HG22	1:A:889:ALA:N	2.16	0.59
1:A:896:VAL:HG21	1:A:901:ALA:O	2.02	0.59
1:A:242:GLY:HA2	1:A:245:LEU:HD12	1.85	0.58
1:A:1087:PHE:CD2	1:A:1091:VAL:HG21	2.37	0.58
1:A:768:LYS:O	1:A:772:GLU:HG3	2.04	0.57
1:A:939:THR:HG23	1:A:945:GLY:CA	2.35	0.57
1:A:779:LEU:HD12	1:A:780:PRO:HD2	1.87	0.57
1:A:498:ASN:HD21	1:A:1040:PRO:HB3	1.70	0.56
1:A:382:PHE:CE2	1:A:398:ARG:HD3	2.40	0.56
1:A:905:GLU:HG2	1:A:993:PHE:CE1	2.40	0.56
1:A:889:ALA:O	1:A:893:GLN:HG3	2.05	0.56
1:A:387:ILE:HD13	1:A:468:LEU:HD12	1.88	0.56
1:A:748:ASP:O	1:A:752:LEU:HD23	2.05	0.55
1:A:509:ASP:OD2	1:A:512:ASN:HB2	2.06	0.55
1:A:1092:LEU:CD1	1:A:1094:ILE:HG13	2.36	0.55
1:A:182:THR:HB	1:A:183:PRO:HD3	1.88	0.55
1:A:800:LYS:HB3	1:A:814:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:LYS:HB2	1:A:814:GLU:HG3	1.90	0.54
1:A:726:THR:HA	1:A:729:LEU:HD12	1.90	0.54
1:A:739:ILE:O	1:A:743:GLN:HG3	2.08	0.54
1:A:1035:LEU:HA	1:A:1039:MET:CG	2.37	0.54
1:A:957:THR:O	1:A:957:THR:HG22	2.08	0.53
1:A:280:TYR:HB3	1:A:282:VAL:HG23	1.89	0.53
1:A:580:TYR:HE2	1:A:613:ARG:HD2	1.72	0.53
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.22	0.53
1:A:775:GLN:HE21	1:A:795:ALA:HB1	1.74	0.52
1:A:996:GLY:O	1:A:1003:SER:HB2	2.09	0.52
1:A:357:CYS:SG	1:A:527:ILE:HD13	2.49	0.52
3:A:1:LXX:C23	3:A:1:LXX:H25	2.37	0.52
1:A:1035:LEU:HD23	1:A:1039:MET:HG3	1.91	0.52
1:A:387:ILE:HD11	1:A:427:ALA:HB1	1.91	0.52
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.45	0.52
1:A:387:ILE:HD13	1:A:468:LEU:CD1	2.40	0.51
1:A:425:LYS:HD2	1:A:672:TYR:OH	2.09	0.51
1:A:759:VAL:HG12	1:A:764:ILE:HG12	1.92	0.51
1:A:393:VAL:O	1:A:393:VAL:HG23	2.11	0.51
1:A:905:GLU:HG2	1:A:993:PHE:CZ	2.46	0.51
1:A:905:GLU:HB3	1:A:909:HIS:CE1	2.46	0.50
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.27	0.50
1:A:280:TYR:HB3	1:A:282:VAL:CG2	2.42	0.50
1:A:293:VAL:HG13	1:A:303:ILE:HD11	1.94	0.50
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.94	0.49
1:A:1035:LEU:CD2	1:A:1039:MET:HG3	2.42	0.49
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.46	0.49
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.94	0.49
1:A:149:ALA:HA	1:A:152:ARG:HD2	1.94	0.49
1:A:607:THR:O	1:A:610:LEU:HB2	2.13	0.49
1:A:939:THR:CG2	1:A:945:GLY:HA2	2.42	0.49
1:A:386:ASN:HB2	1:A:430:ASN:HB3	1.96	0.48
1:A:953:MET:SD	1:A:963:ILE:HD13	2.54	0.48
1:A:683:LYS:HE3	1:A:687:ARG:NH2	2.28	0.48
1:A:377:THR:HG23	1:A:378:ASP:HB3	1.96	0.48
1:A:173:LEU:O	1:A:177:ARG:HG3	2.14	0.48
1:A:148:GLN:O	1:A:152:ARG:HG3	2.14	0.48
1:A:705:GLN:HG3	1:A:839:ARG:CZ	2.44	0.48
1:A:774:LEU:HA	1:A:778:ASN:HB3	1.97	0.47
1:A:373:LEU:HD12	1:A:374:PRO:O	2.14	0.47
1:A:354:LEU:HA	1:A:527:ILE:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:THR:HG23	1:A:945:GLY:HA3	1.97	0.47
1:A:207:LEU:HD23	1:A:212:TRP:CD2	2.50	0.47
1:A:988:THR:HB	1:A:989:PRO:HD2	1.97	0.46
1:A:1042:LEU:HA	1:A:1047:ASP:OD2	2.16	0.45
1:A:377:THR:HA	1:A:378:ASP:HA	1.59	0.45
1:A:224:ILE:HD12	1:A:248:PHE:CD1	2.51	0.45
1:A:1087:PHE:O	1:A:1091:VAL:HB	2.17	0.45
1:A:624:VAL:O	1:A:628:MET:HG2	2.16	0.45
1:A:965:PHE:O	1:A:969:LEU:HG	2.17	0.45
1:A:898:ASN:O	1:A:1087:PHE:HZ	2.00	0.44
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.98	0.44
1:A:916:PRO:HD2	1:A:920:LYS:HD2	1.99	0.44
1:A:589:TYR:O	1:A:593:PHE:HD1	2.00	0.44
1:A:1071:GLN:OE1	1:A:1071:GLN:HA	2.17	0.44
1:A:387:ILE:CG2	1:A:395:CYS:HB3	2.47	0.44
1:A:389:HIS:O	1:A:392:GLN:HB3	2.17	0.44
1:A:410:TRP:O	1:A:412:VAL:HG23	2.18	0.44
1:A:779:LEU:HD12	1:A:780:PRO:CD	2.48	0.44
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.46	0.43
1:A:375:ARG:HD2	1:A:375:ARG:C	2.39	0.43
1:A:774:LEU:O	1:A:778:ASN:HB3	2.18	0.43
1:A:915:SER:OG	1:A:921:PHE:HB2	2.18	0.43
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.99	0.43
1:A:555:LEU:O	1:A:559:ILE:HG13	2.18	0.43
1:A:472:ARG:O	1:A:473:PHE:HB2	2.19	0.43
1:A:366:ARG:NH1	1:A:479:GLU:OE2	2.52	0.43
1:A:282:VAL:HG12	1:A:283:GLY:H	1.84	0.43
1:A:731:ASP:O	1:A:735:GLN:HG3	2.18	0.43
1:A:933:ALA:O	1:A:937:VAL:HG23	2.19	0.43
1:A:380:THR:O	1:A:435:CYS:HA	2.19	0.43
1:A:935:TYR:CE1	1:A:961:PHE:HA	2.54	0.42
1:A:291:GLN:OE1	1:A:291:GLN:HA	2.19	0.42
1:A:378:ASP:O	1:A:379:LEU:HB2	2.19	0.42
1:A:507:ASN:HA	1:A:508:PRO:HD3	1.91	0.42
1:A:809:LYS:N	1:A:810:PRO:HD3	2.34	0.42
1:A:1090:LEU:HD12	1:A:1090:LEU:N	2.34	0.42
1:A:466:LEU:HD11	1:A:476:ARG:HD3	2.00	0.42
1:A:280:TYR:OH	1:A:311:PRO:HG3	2.19	0.42
1:A:899:THR:C	1:A:901:ALA:H	2.23	0.42
1:A:235:VAL:HG21	1:A:244:ILE:HD13	2.02	0.42
1:A:745:VAL:HG12	1:A:811:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:PHE:CD1	1:A:717:LEU:HD11	2.55	0.41
1:A:358:ASP:O	1:A:419:LYS:HG3	2.19	0.41
1:A:424:PRO:HD2	1:A:427:ALA:HB2	2.02	0.41
1:A:640:VAL:O	1:A:643:ILE:HG12	2.21	0.41
1:A:1028:ILE:HG12	1:A:1051:ILE:HG23	2.01	0.41
1:A:422:ASP:HB3	1:A:599:GLY:O	2.21	0.41
1:A:862:LEU:N	1:A:862:LEU:HD22	2.36	0.41
1:A:953:MET:HG3	1:A:963:ILE:HD13	2.01	0.41
1:A:1086:TRP:HE3	1:A:1090:LEU:HD13	1.85	0.41
1:A:1008:LYS:O	1:A:1012:VAL:HG23	2.20	0.41
1:A:233:ILE:HD12	1:A:248:PHE:HD1	1.86	0.41
1:A:310:PRO:HA	1:A:311:PRO:HD3	1.89	0.41
1:A:557:ALA:O	1:A:561:THR:HG23	2.21	0.41
1:A:762:GLN:O	1:A:766:GLN:HG2	2.21	0.41
1:A:706:SER:O	1:A:710:GLN:HB3	2.21	0.41
1:A:1035:LEU:HD12	1:A:1048:ILE:HA	2.04	0.40
1:A:892:GLN:HE22	1:A:1080:TRP:HH2	1.69	0.40
1:A:915:SER:HA	1:A:916:PRO:HD3	1.89	0.40
1:A:605:ALA:O	1:A:609:GLN:HG3	2.21	0.40
1:A:802:LYS:HG3	1:A:812:TRP:HB3	2.03	0.40
1:A:914:LYS:HA	1:A:914:LYS:HD3	1.95	0.40
1:A:1041:GLN:O	1:A:1042:LEU:HD12	2.21	0.40
1:A:783:PHE:CE1	1:A:793:ALA:HB3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	818/966 (85%)	777 (95%)	39 (5%)	2 (0%)	52 64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	896	VAL

5.3.2 Protein sidechains [i](#)

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	751/864 (87%)	735 (98%)	16 (2%)	61	78

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	LEU
1	A	271	VAL
1	A	380	THR
1	A	601	GLN
1	A	763	VAL
1	A	779	LEU
1	A	791	LEU
1	A	832	PHE
1	A	907	LEU
1	A	939	THR
1	A	959	ASN
1	A	983	VAL
1	A	1026	LEU
1	A	1027	LEU
1	A	1039	MET
1	A	1076	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	834	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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$
3	LXX	A	1	-	29,29,29	1.39	5 (17%)	36,41,41	2.22	8 (22%)
2	SO4	A	2	-	4,4,4	0.16	0	6,6,6	0.21	0

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
3	LXX	A	1	-	-	0/8/8/8	0/5/5/5
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	LXX	C17-C18	-2.78	1.44	1.49
3	A	1	LXX	C24-C13	-2.67	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	LXX	C25-C24	-2.20	1.38	1.42
3	A	1	LXX	C12-C13	-2.18	1.37	1.41
3	A	1	LXX	C8-C9	-2.01	1.37	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	LXX	C7-C8-C9	-7.75	107.51	121.44
3	A	1	LXX	C6-N5-C4	-5.81	110.08	116.93
3	A	1	LXX	C9-C1-N2	-3.00	103.93	111.38
3	A	1	LXX	C8-C9-C1	-2.22	123.00	130.94
3	A	1	LXX	C8-C7-C6	2.62	121.35	116.00
3	A	1	LXX	C8-C9-C4	3.58	130.14	118.10
3	A	1	LXX	C7-C6-N5	3.79	130.26	125.46
3	A	1	LXX	C17-C24-C13	3.83	119.46	117.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	LXX	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	837/966 (86%)	0.71	106 (12%) 5 8	25, 56, 110, 174	1 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	777	LEU	13.5
1	A	377	THR	13.1
1	A	378	ASP	8.9
1	A	375	ARG	8.2
1	A	229	THR	7.7
1	A	374	PRO	7.3
1	A	376	ASN	7.2
1	A	143	MET	6.4
1	A	228	THR	6.3
1	A	379	LEU	6.2
1	A	898	ASN	6.1
1	A	895	THR	5.8
1	A	270	PHE	5.7
1	A	148	GLN	5.7
1	A	231	GLN	5.5
1	A	531	LYS	5.1
1	A	778	ASN	5.1
1	A	227	SER	5.1
1	A	234	LYS	4.7
1	A	661	LEU	4.5
1	A	248	PHE	4.4
1	A	1094	ILE	4.3
1	A	657	LEU	4.2
1	A	1091	VAL	4.2
1	A	779	LEU	4.2
1	A	843	LEU	4.0
1	A	230	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	664	VAL	3.9
1	A	353	SER	3.9
1	A	354	LEU	3.8
1	A	758	ASP	3.8
1	A	896	VAL	3.8
1	A	774	LEU	3.8
1	A	999	GLY	3.7
1	A	147	SER	3.7
1	A	694	PHE	3.6
1	A	373	LEU	3.5
1	A	823	LEU	3.4
1	A	250	THR	3.4
1	A	660	LEU	3.3
1	A	216	ALA	3.3
1	A	656	VAL	3.2
1	A	744	LYS	3.2
1	A	842	MET	3.2
1	A	698	PHE	3.1
1	A	903	LYS	3.1
1	A	663	LEU	3.1
1	A	226	ARG	3.1
1	A	870	ILE	3.1
1	A	245	LEU	3.1
1	A	666	ALA	3.0
1	A	150	PHE	3.0
1	A	869	CYS	3.0
1	A	695	LEU	3.0
1	A	846	GLN	3.0
1	A	237	PRO	2.9
1	A	899	THR	2.9
1	A	762	GLN	2.9
1	A	221	PHE	2.8
1	A	529	LEU	2.8
1	A	667	VAL	2.7
1	A	780	PRO	2.7
1	A	232	THR	2.7
1	A	747	LEU	2.7
1	A	845	LEU	2.7
1	A	844	ILE	2.7
1	A	307	LEU	2.6
1	A	320	LYS	2.6
1	A	1037	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1030	LEU	2.6
1	A	759	VAL	2.6
1	A	355	TRP	2.6
1	A	244	ILE	2.5
1	A	681	LEU	2.5
1	A	213	LYS	2.5
1	A	659	TYR	2.5
1	A	850	ILE	2.4
1	A	658	HIS	2.4
1	A	662	GLN	2.4
1	A	787	TYR	2.4
1	A	214	LYS	2.4
1	A	763	VAL	2.3
1	A	246	GLN	2.3
1	A	865	LEU	2.3
1	A	217	ASN	2.3
1	A	894	SER	2.3
1	A	982	ARG	2.3
1	A	665	GLN	2.2
1	A	212	TRP	2.2
1	A	847	ILE	2.2
1	A	631	LEU	2.2
1	A	381	VAL	2.2
1	A	152	ARG	2.2
1	A	871	SER	2.2
1	A	692	GLY	2.1
1	A	1062	GLU	2.1
1	A	1001	LYS	2.1
1	A	902	PHE	2.1
1	A	867	TYR	2.1
1	A	1034	MET	2.1
1	A	848	LEU	2.1
1	A	372	VAL	2.1
1	A	628	MET	2.0
1	A	1002	THR	2.0
1	A	699	LEU	2.0
1	A	403	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	2	5/5	0.99	0.14	1.29	39,49,56,56	0
3	LXX	A	1	25/25	0.90	0.15	-0.52	46,67,75,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.