



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:29 AM GMT

PDB ID : 3LVG
Title : Crystal structure of a clathrin heavy chain and clathrin light chain complex
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Deposited on : 2010-02-20
Resolution : 7.94 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

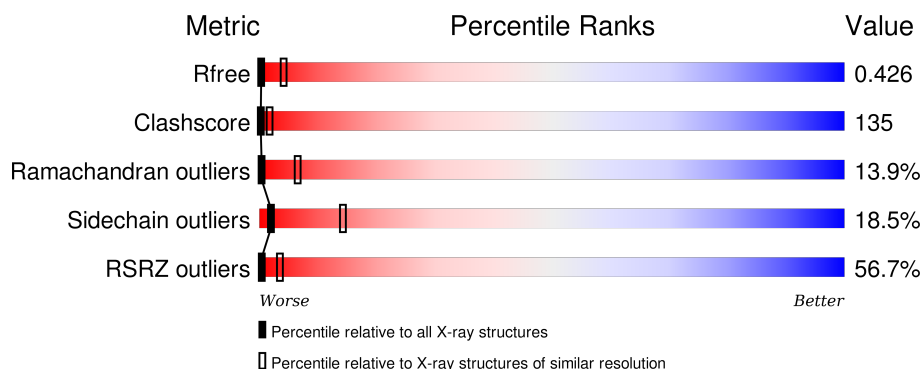
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.94 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	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	624	<div> <div>55%</div> <div>14% 49% 21% 6% 11%</div> </div>
1	B	624	<div> <div>59%</div> <div>12% 52% 20% 5% 11%</div> </div>
1	C	624	<div> <div>38%</div> <div>13% 50% 20% 6% 11%</div> </div>
2	D	190	<div> <div>33%</div> <div>35% 46% 12% 5%</div> </div>
2	E	190	<div> <div>14%</div> <div>16% 32% 9% 39%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	190	<p>17% 18% 36% 13% 31%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16504 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 Clathrin heavy chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4543	2896	767	855	25			
1	B	553	Total	C	N	O	S	0	0	0
			4543	2896	767	855	25			
1	C	553	Total	C	N	O	S	0	0	0
			4543	2896	767	855	25			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	MET	-	EXPRESSION TAG	UNP P49951
A	1053	GLY	-	EXPRESSION TAG	UNP P49951
A	1054	SER	-	EXPRESSION TAG	UNP P49951
A	1055	SER	-	EXPRESSION TAG	UNP P49951
A	1056	HIS	-	EXPRESSION TAG	UNP P49951
A	1057	HIS	-	EXPRESSION TAG	UNP P49951
A	1058	HIS	-	EXPRESSION TAG	UNP P49951
A	1059	HIS	-	EXPRESSION TAG	UNP P49951
A	1060	HIS	-	EXPRESSION TAG	UNP P49951
A	1061	HIS	-	EXPRESSION TAG	UNP P49951
A	1062	SER	-	EXPRESSION TAG	UNP P49951
A	1063	SER	-	EXPRESSION TAG	UNP P49951
A	1064	GLY	-	EXPRESSION TAG	UNP P49951
A	1065	LEU	-	EXPRESSION TAG	UNP P49951
A	1066	VAL	-	EXPRESSION TAG	UNP P49951
A	1067	PRO	-	EXPRESSION TAG	UNP P49951
A	1068	ARG	-	EXPRESSION TAG	UNP P49951
A	1069	GLY	-	EXPRESSION TAG	UNP P49951
A	1070	SER	-	EXPRESSION TAG	UNP P49951
A	1071	HIS	-	EXPRESSION TAG	UNP P49951
A	1072	MET	-	EXPRESSION TAG	UNP P49951
A	1073	LEU	-	EXPRESSION TAG	UNP P49951
B	1052	MET	-	EXPRESSION TAG	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1053	GLY	-	EXPRESSION TAG	UNP P49951
B	1054	SER	-	EXPRESSION TAG	UNP P49951
B	1055	SER	-	EXPRESSION TAG	UNP P49951
B	1056	HIS	-	EXPRESSION TAG	UNP P49951
B	1057	HIS	-	EXPRESSION TAG	UNP P49951
B	1058	HIS	-	EXPRESSION TAG	UNP P49951
B	1059	HIS	-	EXPRESSION TAG	UNP P49951
B	1060	HIS	-	EXPRESSION TAG	UNP P49951
B	1061	HIS	-	EXPRESSION TAG	UNP P49951
B	1062	SER	-	EXPRESSION TAG	UNP P49951
B	1063	SER	-	EXPRESSION TAG	UNP P49951
B	1064	GLY	-	EXPRESSION TAG	UNP P49951
B	1065	LEU	-	EXPRESSION TAG	UNP P49951
B	1066	VAL	-	EXPRESSION TAG	UNP P49951
B	1067	PRO	-	EXPRESSION TAG	UNP P49951
B	1068	ARG	-	EXPRESSION TAG	UNP P49951
B	1069	GLY	-	EXPRESSION TAG	UNP P49951
B	1070	SER	-	EXPRESSION TAG	UNP P49951
B	1071	HIS	-	EXPRESSION TAG	UNP P49951
B	1072	MET	-	EXPRESSION TAG	UNP P49951
B	1073	LEU	-	EXPRESSION TAG	UNP P49951
C	1052	MET	-	EXPRESSION TAG	UNP P49951
C	1053	GLY	-	EXPRESSION TAG	UNP P49951
C	1054	SER	-	EXPRESSION TAG	UNP P49951
C	1055	SER	-	EXPRESSION TAG	UNP P49951
C	1056	HIS	-	EXPRESSION TAG	UNP P49951
C	1057	HIS	-	EXPRESSION TAG	UNP P49951
C	1058	HIS	-	EXPRESSION TAG	UNP P49951
C	1059	HIS	-	EXPRESSION TAG	UNP P49951
C	1060	HIS	-	EXPRESSION TAG	UNP P49951
C	1061	HIS	-	EXPRESSION TAG	UNP P49951
C	1062	SER	-	EXPRESSION TAG	UNP P49951
C	1063	SER	-	EXPRESSION TAG	UNP P49951
C	1064	GLY	-	EXPRESSION TAG	UNP P49951
C	1065	LEU	-	EXPRESSION TAG	UNP P49951
C	1066	VAL	-	EXPRESSION TAG	UNP P49951
C	1067	PRO	-	EXPRESSION TAG	UNP P49951
C	1068	ARG	-	EXPRESSION TAG	UNP P49951
C	1069	GLY	-	EXPRESSION TAG	UNP P49951
C	1070	SER	-	EXPRESSION TAG	UNP P49951
C	1071	HIS	-	EXPRESSION TAG	UNP P49951
C	1072	MET	-	EXPRESSION TAG	UNP P49951

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1073	LEU	-	EXPRESSION TAG	UNP P49951

- Molecule 2 is a protein called Clathrin light chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	180	Total	C	N	O	S	0	0	0
			1146	690	227	228	1			
2	E	116	Total	C	N	O	S	0	0	0
			823	497	163	162	1			
2	F	132	Total	C	N	O	S	0	0	0
			906	546	179	180	1			

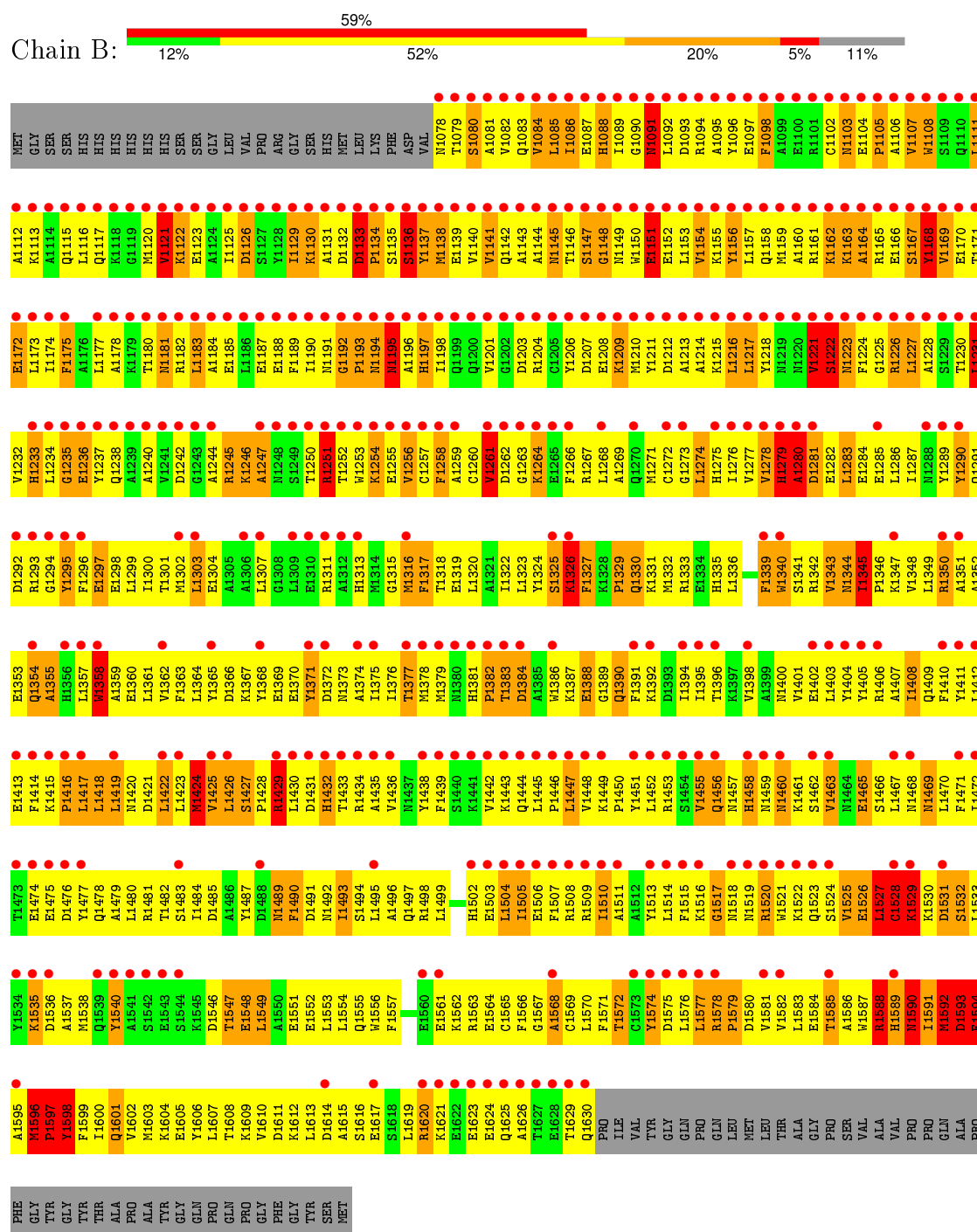
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

- Chain A:

Category	Item	Value	Color
P1597	P1597	14%	Green
	P1598	14%	Green
	P1599	14%	Green
	P1600	14%	Green
	Q1601	14%	Green
	V1602	14%	Green
	M1603	14%	Green
	K1604	14%	Green
	E1605	14%	Green
	V1606	14%	Green
P1607	P1607	14%	Green
	M1608	14%	Green
	K1609	14%	Green
	V1610	14%	Green
	E1611	14%	Green
	K1612	14%	Green
	V1613	14%	Green
	E1614	14%	Green
	V1615	14%	Green
	E1616	14%	Green
P1617	P1617	14%	Green
	M1618	14%	Green
	K1619	14%	Green
	V1620	14%	Green
	E1621	14%	Green
	K1622	14%	Green
	V1623	14%	Green
	E1624	14%	Green
	V1625	14%	Green
	E1626	14%	Green
P1627	P1627	14%	Green
	M1628	14%	Green
	K1629	14%	Green
	V1630	14%	Green
	E1631	14%	Green
	K1632	14%	Green
	V1633	14%	Green
	E1634	14%	Green
	V1635	14%	Green
	E1636	14%	Green
P1637	P1637	14%	Green
	M1638	14%	Green
	K1639	14%	Green
	V1640	14%	Green
	E1641	14%	Green
	K1642	14%	Green
	V1643	14%	Green
	E1644	14%	Green
	V1645	14%	Green
	E1646	14%	Green
P1647	P1647	14%	Green
	M1648	14%	Green
	K1649	14%	Green
	V1650	14%	Green
	E1651	14%	Green
	K1652	14%	Green
	V1653	14%	Green
	E1654	14%	Green
	V1655	14%	Green
	E1656	14%	Green
P1657	P1657	14%	Green
	M1658	14%	Green
	K1659	14%	Green
	V1660	14%	Green
	E1661	14%	Green
	K1662	14%	Green
	V1663	14%	Green
	E1664	14%	Green
	V1665	14%	Green
	E1666	14%	Green
P1667	P1667	14%	Green
	M1668	14%	Green
	K1669	14%	Green
	V1670	14%	Green
	E1671	14%	Green
	K1672	14%	Green
	V1673	14%	Green
	E1674	14%	Green
	V1675	14%	Green
	E1676	14%	Green
P1677	P1677	14%	Green
	M1678	14%	Green
	K1679	14%	Green
	V1680	14%	Green
	E1681	14%	Green
	K1682	14%	Green
	V1683	14%	Green
	E1684	14%	Green
	V1685	14%	Green
	E1686	14%	Green
P1687	P1687	14%	Green
	M1688	14%	Green
	K1689	14%	Green
	V1690	14%	Green
	E1691	14%	Green
	K1692	14%	Green
	V1693	14%	Green
	E1694	14%	Green
	V1695	14%	Green
	E1696	14%	Green
P1697	P1697	14%	Green
	M1698	14%	Green
	K1699	14%	Green
	V1700	14%	Green
	E1701	14%	Green
	K1702	14%	Green
	V1703	14%	Green
	E1704	14%	Green
	V1705	14%	Green
	E1706	14%	Green
P1707	P1707	14%	Green
	M1708	14%	Green
	K1709	14%	Green
	V1710	14%	Green
	E1711	14%	Green
	K1712	14%	Green
	V1713	14%	Green
	E1714	14%	Green
	V1715	14%	Green
	E1716	14%	Green
P1717	P1717	14%	Green
	M1718	14%	Green
	K1719	14%	Green
	V1720	14%	Green
	E1721	14%	Green
	K1722	14%	Green
	V1723	14%	Green
	E1724	14%	Green
	V1725	14%	Green
	E1726	14%	Green
P1727	P1727	14%	Green
	M1728	14%	Green
	K1729	14%	Green
	V1730	14%	Green
	E1731	14%	Green
	K1732	14%	Green
	V1733	14%	Green
	E1734	14%	Green
	V1735	14%	Green

TYR
GLY
THR
ALA
PRO
ALA
TYR
GLY
GLN
PRO
GLN
GLY
PHE
GLY
TYR
SER
MET

• Molecule 1: Clathrin heavy chain 1



- Molecule 2: Clathrin light chain B

Response	Percentage
U.S. is a threat	33%
U.S. is not a threat	35%
U.S. is a threat	46%
U.S. is not a threat	12%
U.S. is a threat	5%





4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	228.56 Å 228.56 Å 710.32 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 7.94 82.22 – 4.99	Depositor EDS
% Data completeness (in resolution range)	99.6 (100.00-7.94) 63.0 (82.22-4.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 5.12 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.419 , 0.425 0.423 , 0.426	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	310.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 471.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 26103 reflections	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	16504	wwPDB-VP
Average B, all atoms (Å ²)	295.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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 i

5.1 Standard geometry i

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	0.83	20/4638 (0.4%)	1.27	83/6266 (1.3%)
1	B	0.80	17/4638 (0.4%)	1.26	83/6266 (1.3%)
1	C	0.77	13/4638 (0.3%)	1.20	73/6266 (1.2%)
2	D	0.75	0/647	1.15	8/866 (0.9%)
2	E	0.69	0/589	1.24	5/785 (0.6%)
2	F	0.77	0/642	1.20	8/859 (0.9%)
All	All	0.79	50/15792 (0.3%)	1.24	260/21308 (1.2%)

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	1	8
1	B	0	3
1	C	2	3
2	F	0	1
All	All	3	15

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1162	LYS	C-O	-19.68	0.85	1.23
1	A	1222	SER	C-O	18.12	1.57	1.23
1	C	1182	ARG	C-O	17.19	1.56	1.23
1	C	1136	SER	C-O	-17.10	0.90	1.23
1	C	1248	ASN	N-CA	17.04	1.80	1.46

The worst 5 of 260 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1162	LYS	CA-C-O	22.12	166.55	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1279	HIS	O-C-N	-22.04	87.43	122.70
1	C	1223	ASN	N-CA-C	18.52	161.00	111.00
1	A	1103	ASN	C-N-CA	-17.51	77.93	121.70
1	A	1162	LYS	O-C-N	-16.77	95.87	122.70

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1104	GLU	CA
1	C	1137	TYR	CA
1	C	1223	ASN	CA

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1103	ASN	Mainchain
1	A	1104	GLU	Mainchain
1	A	1133	ASP	Mainchain
1	A	1147	SER	Mainchain
1	A	1162	LYS	Mainchain

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	4543	0	4454	1296	1
1	B	4543	0	4456	1248	3
1	C	4543	0	4455	1291	4
2	D	1146	0	735	252	0
2	E	823	0	633	246	0
2	F	906	0	669	239	0
All	All	16504	0	15402	4313	5

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 135.

The worst 5 of 4313 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:1258:PHE:HB2	1:A:1289:TYR:CD2	1.19	1.69
1:A:1253:TRP:CZ3	1:A:1276:ILE:HG22	1.25	1.64
1:C:1253:TRP:CZ3	1:C:1276:ILE:HG22	1.25	1.64
1:A:1258:PHE:CB	1:A:1289:TYR:CE2	1.75	1.63
1:B:1253:TRP:CZ3	1:B:1276:ILE:HG22	1.25	1.63

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1340:TRP:CZ2	1:C:1222:SER:OG[12_655]	1.80	0.40
1:C:1304:GLU:OE2	1:C:1334:GLU:OE2[15_645]	1.98	0.22
1:A:1199:GLN:NE2	1:A:1431:ASP:OD2[10_555]	2.13	0.07
1:B:1340:TRP:CZ2	1:C:1222:SER:CB[12_655]	2.15	0.05
1:B:1341:SER:OG	1:C:1203:ASP:OD2[12_655]	2.18	0.02

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	551/624 (88%)	322 (58%)	152 (28%)	77 (14%)	0	6
1	B	551/624 (88%)	319 (58%)	161 (29%)	71 (13%)	0	7
1	C	551/624 (88%)	309 (56%)	164 (30%)	78 (14%)	0	6
2	D	77/190 (40%)	50 (65%)	16 (21%)	11 (14%)	0	6
2	E	66/190 (35%)	35 (53%)	21 (32%)	10 (15%)	0	5
2	F	76/190 (40%)	42 (55%)	20 (26%)	14 (18%)	0	4
All	All	1872/2442 (77%)	1077 (58%)	534 (28%)	261 (14%)	0	6

5 of 261 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1087	GLU
1	A	1091	ASN
1	A	1105	PRO
1	A	1122	LYS
1	A	1130	LYS

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	485/541 (90%)	409 (84%)	76 (16%)	3	21
1	B	485/541 (90%)	404 (83%)	81 (17%)	3	19
1	C	485/541 (90%)	395 (81%)	90 (19%)	2	14
2	D	62/73 (85%)	45 (73%)	17 (27%)	0	4
2	E	61/73 (84%)	42 (69%)	19 (31%)	0	2
2	F	62/73 (85%)	42 (68%)	20 (32%)	0	2
All	All	1640/1842 (89%)	1337 (82%)	303 (18%)	2	14

5 of 303 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1527	LEU
1	C	1108	TRP
2	E	140	GLN
1	B	1549	LEU
1	B	1601	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1390	GLN
1	B	1523	GLN
2	D	153	ASN
1	B	1456	GLN

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Mol	Chain	Res	Type
1	B	1468	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 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, 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	553/624 (88%)	4.12	342 (61%) 0 3	306, 348, 348, 348	0
1	B	553/624 (88%)	4.91	368 (66%) 0 3	257, 257, 318, 319	0
1	C	553/624 (88%)	2.81	238 (43%) 0 4	232, 232, 308, 309	0
2	D	79/190 (41%)	4.22	62 (78%) 0 2	298, 298, 298, 298	0
2	E	68/190 (35%)	1.97	26 (38%) 0 4	314, 314, 314, 314	0
2	F	78/190 (41%)	3.16	33 (42%) 0 4	339, 339, 339, 339	0
All	All	1884/2442 (77%)	3.85	1069 (56%) 0 3	232, 307, 348, 348	0

The worst 5 of 1069 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1091	ASN	38.3
1	C	1078	ASN	36.0
1	C	1090	GLY	34.7
1	C	1079	THR	33.3
1	B	1106	ALA	29.6

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.