Full wwPDB X-ray Structure Validation Report

Jun 2, 2016 – 06:49 PM EDT

PDB ID	:	5AAA
Title	:	Structure of L1198F Mutant Human Anaplastic Lymphoma Kinase in Complex with Crizotinib
Authors	:	McTigue, M.; Deng, Y.; Liu, W.; Brooun, A.; Stewart, A.
Deposited on	:	2015-07-23
Resolution	:	1.73 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

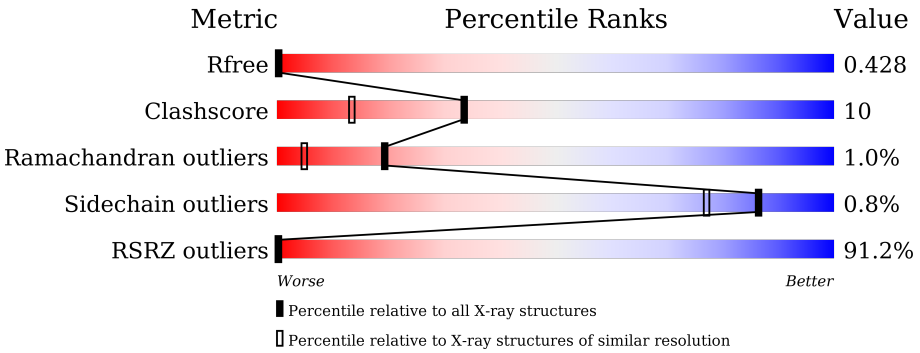
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.73 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	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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 <=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	327	82% 76% 13% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2607 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.

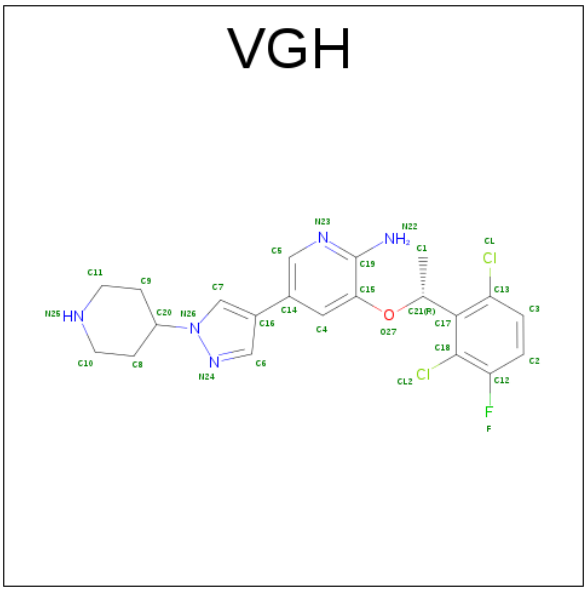
- Molecule 1 is a protein called ALK TYROSINE KINASE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	4	1
			2350	1498	401	428	23			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1085	MET	-	EXPRESSION TAG	UNP Q9UM73
A	1086	ALA	-	EXPRESSION TAG	UNP Q9UM73
A	1087	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1088	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1089	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1090	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1091	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1092	HIS	-	EXPRESSION TAG	UNP Q9UM73
A	1198	PHE	LEU	ENGINEERED MUTATION	UNP Q9UM73

- Molecule 2 is 3-[(1R)-1-(2,6-DICHLORO-3-FLUOROPHENYL)ETHOXY]-5-(1-PIPERIDIN-4-YL-1H-PYRAZOL-4-YL)PYRIDIN-2-AMINE (three-letter code: VGH) (formula: $C_{21}H_{22}Cl_2FN_5O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			30	21	2	1	5	1		

- Molecule 3 is water.

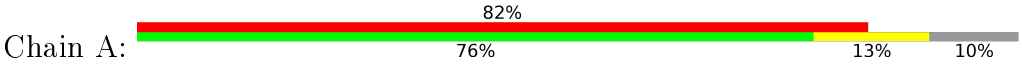
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	227	Total	O	0	0
			227	227		

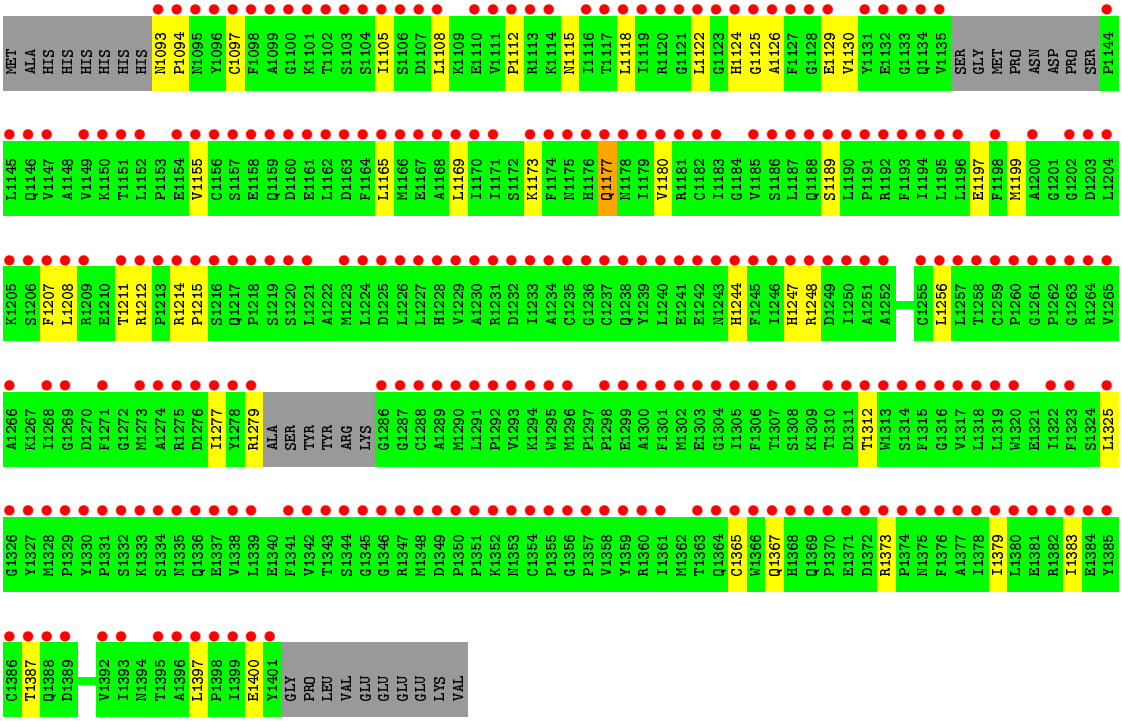
3 Residue-property plots (i)

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 (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: ALK TYROSINE KINASE RECEPTOR

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.47Å 57.28Å 104.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.35 – 1.73 50.25 – 2.02	Depositor EDS
% Data completeness (in resolution range)	89.5 (52.35-1.73) 95.7 (50.25-2.02)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.01Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.200 , 0.206 0.420 , 0.428	Depositor DCC
R_{free} test set	590 reflections (2.92%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.76	EDS
Total number of atoms	2607	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: VGH

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	0.26	0/2408	0.45	0/3263

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	2350	0	2317	47	0
2	A	30	0	22	3	0
3	A	227	0	0	4	0
All	All	2607	0	2339	48	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 10.

All (48) 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:1105:ILE:HD12	1:A:1105:ILE:H	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:HIS:HB3	1:A:1129:GLU:HA	1.56	0.87
1:A:1105:ILE:HG13	1:A:1165:LEU:HD11	1.61	0.81
1:A:1105:ILE:CD1	1:A:1105:ILE:H	1.94	0.81
1:A:1105:ILE:HD12	1:A:1105:ILE:N	2.00	0.75
1:A:1093:ASN:HB2	1:A:1105:ILE:HD13	1.69	0.74
1:A:1214:ARG:HG3	1:A:1215:PRO:HD2	1.69	0.74
1:A:1165:LEU:O	1:A:1169:LEU:HD13	1.95	0.66
1:A:1248:ARG:CZ	1:A:1277:ILE:HG21	2.25	0.65
1:A:1279:ARG:HE	1:A:1279:ARG:HA	1.60	0.65
1:A:1367:GLN:O	1:A:1373:ARG:HD3	1.98	0.63
1:A:1093:ASN:HB2	1:A:1105:ILE:CD1	2.29	0.62
1:A:1097[A]:CYS:HB3	3:A:2029:HOH:O	2.00	0.62
1:A:1155:VAL:O	1:A:1155:VAL:HG23	2.02	0.59
1:A:1367:GLN:HB2	1:A:1373:ARG:HG2	1.85	0.58
1:A:1244:HIS:HD2	3:A:2008:HOH:O	1.86	0.58
1:A:1279:ARG:NE	1:A:1279:ARG:HA	2.19	0.57
1:A:1248:ARG:NH1	1:A:1277:ILE:HG21	2.20	0.57
1:A:1177:GLN:NE2	1:A:1177:GLN:H	2.03	0.57
1:A:1199:MET:HA	1:A:1199:MET:HE2	1.87	0.57
1:A:1105:ILE:HG13	1:A:1165:LEU:CD1	2.32	0.55
1:A:1112:PRO:HG2	1:A:1115:ASN:OD1	2.06	0.55
1:A:1180:VAL:HG21	1:A:1256:LEU:HD12	1.89	0.55
1:A:1097[B]:CYS:HB2	3:A:2029:HOH:O	2.07	0.54
1:A:1208:LEU:O	1:A:1212:ARG:HG3	2.08	0.54
1:A:1365:CYS:O	1:A:1373:ARG:HD2	2.07	0.53
1:A:1197:GLU:HG2	1:A:1199:MET:HE3	1.91	0.53
1:A:1093:ASN:HD22	1:A:1105:ILE:HD13	1.75	0.52
1:A:1199:MET:CE	1:A:1199:MET:HA	2.42	0.49
1:A:1256:LEU:HD11	2:A:9000:VGH:CL2	2.50	0.49
1:A:1108:LEU:HD11	1:A:1169:LEU:CD1	2.43	0.48
1:A:1247:HIS:O	1:A:1248:ARG:HB2	2.14	0.47
1:A:1197:GLU:HG2	1:A:1199:MET:CE	2.44	0.47
2:A:9000:VGH:CL2	2:A:9000:VGH:H12C	2.52	0.47
1:A:1207:PHE:O	1:A:1211:THR:HG22	2.16	0.46
1:A:1124:HIS:CD2	1:A:1129:GLU:HB3	2.51	0.45
1:A:1383:ILE:O	1:A:1387:THR:HG23	2.18	0.43
1:A:1325:LEU:HD22	1:A:1325:LEU:N	2.34	0.42
1:A:1180:VAL:HG13	1:A:1197:GLU:HB3	2.01	0.41
1:A:1199:MET:O	2:A:9000:VGH:H5	2.20	0.41
1:A:1093:ASN:HA	1:A:1094:PRO:HD3	1.84	0.41
1:A:1169:LEU:O	1:A:1173:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:SER:N	3:A:2037:HOH:O	2.50	0.41
1:A:1214:ARG:HG3	1:A:1215:PRO:CD	2.46	0.41
1:A:1122:LEU:HD12	1:A:1130:VAL:HG12	2.03	0.41
1:A:1108:LEU:HD21	1:A:1169:LEU:HD12	2.02	0.41
1:A:1325:LEU:HD21	1:A:1397:LEU:HD22	2.01	0.41
1:A:1312:THR:HG23	1:A:1379:ILE:HD11	2.03	0.41

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	293/327 (90%)	281 (96%)	9 (3%)	3 (1%)	19 5

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1126	ALA
1	A	1400	GLU
1	A	1125	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	260/285 (91%)	258 (99%)	2 (1%)	86 77

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1118	LEU
1	A	1177	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1093	ASN
1	A	1115	ASN
1	A	1124	HIS
1	A	1177	GLN
1	A	1188	GLN
1	A	1217	GLN
1	A	1238	GLN
1	A	1243	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 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	VGH	A	9000	-	29,33,33	2.46	12 (41%)	31,47,47	1.68	6 (19%)

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	VGH	A	9000	-	-	0/12/24/24	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	9000	VGH	N24-N26	-5.29	1.29	1.35
2	A	9000	VGH	C6-N24	-2.41	1.29	1.33
2	A	9000	VGH	C4-C14	2.10	1.43	1.39
2	A	9000	VGH	C2-C12	2.13	1.42	1.37
2	A	9000	VGH	C5-C14	2.28	1.43	1.39
2	A	9000	VGH	C17-C21	2.37	1.57	1.53
2	A	9000	VGH	C19-N22	2.83	1.41	1.34
2	A	9000	VGH	O27-C21	3.15	1.47	1.42
2	A	9000	VGH	C4-C15	3.16	1.44	1.38
2	A	9000	VGH	C13-C17	4.60	1.46	1.39
2	A	9000	VGH	C18-C17	5.00	1.47	1.39
2	A	9000	VGH	C7-N26	5.03	1.41	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	9000	VGH	C16-C7-N26	-4.34	104.04	109.80
2	A	9000	VGH	C1-C21-C17	-2.29	110.76	113.34
2	A	9000	VGH	C13-C17-C18	2.13	118.09	114.95
2	A	9000	VGH	C17-C18-CL2	2.89	123.06	120.34
2	A	9000	VGH	C17-C13-CL	2.97	123.46	120.43
2	A	9000	VGH	C15-O27-C21	5.09	126.12	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	9000	VGH	3	0

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, 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	295/327 (90%)	5.10	269 (91%)	0	14, 26, 56, 72	0

All (269) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1401	TYR	28.5
1	A	1105	ILE	26.2
1	A	1279	ARG	18.9
1	A	1278	TYR	16.4
1	A	1286	GLY	15.2
1	A	1093	ASN	14.9
1	A	1169	LEU	14.4
1	A	1400	GLU	14.2
1	A	1127	PHE	13.5
1	A	1098	PHE	13.0
1	A	1096[A]	TYR	12.9
1	A	1326	GLY	12.4
1	A	1094	PRO	11.8
1	A	1187	LEU	11.7
1	A	1399	ILE	11.0
1	A	1273	MET	10.8
1	A	1097[A]	CYS	10.7
1	A	1165	LEU	10.5
1	A	1125	GLY	10.4
1	A	1100	GLY	10.0
1	A	1145	LEU	9.9
1	A	1102	THR	9.9
1	A	1214	ARG	9.9
1	A	1256	LEU	9.5
1	A	1193	PHE	9.2
1	A	1219	SER	9.1
1	A	1217	GLN	8.8

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Mol	Chain	Res	Type	RSRZ
1	A	1168	ALA	8.8
1	A	1274	ALA	8.6
1	A	1322	ILE	8.6
1	A	1215	PRO	8.3
1	A	1328	MET	8.3
1	A	1189	SER	8.3
1	A	1119	ILE	8.3
1	A	1101	LYS	8.3
1	A	1155	VAL	8.1
1	A	1218	PRO	7.9
1	A	1346	GLY	7.9
1	A	1325	LEU	7.8
1	A	1287	GLY	7.8
1	A	1327	TYR	7.8
1	A	1149	VAL	7.8
1	A	1358	VAL	7.5
1	A	1131	TYR	7.5
1	A	1211	THR	7.4
1	A	1385	TYR	7.4
1	A	1099	ALA	7.4
1	A	1271	PHE	7.4
1	A	1277	ILE	7.3
1	A	1124	HIS	7.3
1	A	1194	ILE	7.2
1	A	1247	HIS	7.2
1	A	1207	PHE	7.2
1	A	1380	LEU	7.2
1	A	1095	ASN	7.1
1	A	1339	LEU	7.1
1	A	1164	PHE	7.1
1	A	1376	PHE	7.1
1	A	1307	THR	7.0
1	A	1190	LEU	6.9
1	A	1174	PHE	6.9
1	A	1126	ALA	6.8
1	A	1317	VAL	6.8
1	A	1248	ARG	6.7
1	A	1122	LEU	6.5
1	A	1135	VAL	6.5
1	A	1263	GLY	6.5
1	A	1348	MET	6.5
1	A	1118	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	1258	THR	6.4
1	A	1220	SER	6.3
1	A	1144	PRO	6.2
1	A	1120	ARG	6.2
1	A	1268	ILE	6.1
1	A	1361	ILE	6.1
1	A	1150	LYS	6.1
1	A	1341	PHE	6.1
1	A	1114	LYS	6.1
1	A	1398	PRO	6.0
1	A	1200	ALA	6.0
1	A	1203	ASP	6.0
1	A	1233	ILE	6.0
1	A	1108	LEU	5.9
1	A	1303	GLU	5.8
1	A	1208	LEU	5.8
1	A	1378	ILE	5.7
1	A	1353	ASN	5.6
1	A	1319	LEU	5.5
1	A	1237	CYS	5.5
1	A	1245	PHE	5.5
1	A	1333	LYS	5.5
1	A	1379	ILE	5.4
1	A	1320	TRP	5.4
1	A	1396	ALA	5.4
1	A	1302	MET	5.4
1	A	1289	ALA	5.4
1	A	1121	GLY	5.4
1	A	1179	ILE	5.3
1	A	1292	PRO	5.3
1	A	1393	ILE	5.3
1	A	1198	PHE	5.3
1	A	1330	TYR	5.3
1	A	1250	ILE	5.3
1	A	1301	PHE	5.3
1	A	1221	LEU	5.3
1	A	1229	VAL	5.2
1	A	1132	GLU	5.2
1	A	1192	ARG	5.2
1	A	1313	TRP	5.2
1	A	1224	LEU	5.2
1	A	1397	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	1239	TYR	5.2
1	A	1369	GLN	5.2
1	A	1323	PHE	5.1
1	A	1387	THR	5.1
1	A	1276	ASP	5.1
1	A	1305	ILE	5.1
1	A	1315	PHE	5.1
1	A	1204	LEU	5.0
1	A	1128	GLY	5.0
1	A	1359	TYR	4.9
1	A	1157	SER	4.9
1	A	1306	PHE	4.8
1	A	1156	CYS	4.8
1	A	1180	VAL	4.8
1	A	1261	GLY	4.8
1	A	1171	ILE	4.7
1	A	1111	VAL	4.7
1	A	1213	PRO	4.7
1	A	1191	PRO	4.7
1	A	1265	VAL	4.7
1	A	1243	ASN	4.7
1	A	1185	VAL	4.7
1	A	1363	THR	4.7
1	A	1314	SER	4.7
1	A	1173	LYS	4.6
1	A	1183	ILE	4.6
1	A	1117	THR	4.6
1	A	1216	SER	4.6
1	A	1146	GLN	4.6
1	A	1342	VAL	4.6
1	A	1195	LEU	4.5
1	A	1252	ALA	4.5
1	A	1166	MET	4.5
1	A	1360	ARG	4.4
1	A	1357	PRO	4.4
1	A	1370	PRO	4.4
1	A	1275	ARG	4.4
1	A	1336	GLN	4.3
1	A	1364[A]	GLN	4.3
1	A	1374	PRO	4.3
1	A	1161	GLU	4.2
1	A	1103	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1338	VAL	4.2
1	A	1236	GLY	4.2
1	A	1351	PRO	4.1
1	A	1182	CYS	4.1
1	A	1386	CYS	4.1
1	A	1230	ALA	4.1
1	A	1260	PRO	4.1
1	A	1209	ARG	4.1
1	A	1266	ALA	4.1
1	A	1350	PRO	4.1
1	A	1257	LEU	4.0
1	A	1170	ILE	4.0
1	A	1234	ALA	4.0
1	A	1226	LEU	4.0
1	A	1262	PRO	4.0
1	A	1318	LEU	3.9
1	A	1334	SER	3.9
1	A	1310	THR	3.9
1	A	1295	TRP	3.9
1	A	1371	GLU	3.9
1	A	1186	SER	3.9
1	A	1288	CYS	3.9
1	A	1196	LEU	3.8
1	A	1188	GLN	3.8
1	A	1296	MET	3.8
1	A	1162	LEU	3.8
1	A	1235[A]	CYS	3.8
1	A	1151	THR	3.7
1	A	1337	GLU	3.7
1	A	1212	ARG	3.7
1	A	1298	PRO	3.6
1	A	1352	LYS	3.6
1	A	1345	GLY	3.6
1	A	1158	GLU	3.6
1	A	1392	VAL	3.6
1	A	1251	ALA	3.6
1	A	1225	ASP	3.6
1	A	1384	GLU	3.6
1	A	1227	LEU	3.6
1	A	1238	GLN	3.5
1	A	1300	ALA	3.5
1	A	1246	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1395	THR	3.4
1	A	1349	ASP	3.4
1	A	1106	SER	3.4
1	A	1366	TRP	3.4
1	A	1259	CYS	3.3
1	A	1206	SER	3.3
1	A	1308	SER	3.3
1	A	1343	THR	3.2
1	A	1129	GLU	3.2
1	A	1133	GLY	3.2
1	A	1335	ASN	3.2
1	A	1123	GLY	3.2
1	A	1244	HIS	3.2
1	A	1232	ASP	3.1
1	A	1377	ALA	3.1
1	A	1293	VAL	3.1
1	A	1167	GLU	3.1
1	A	1113	ARG	3.1
1	A	1344	SER	3.1
1	A	1291	LEU	3.1
1	A	1231	ARG	3.1
1	A	1175	ASN	3.1
1	A	1163	ASP	3.1
1	A	1134	GLN	3.0
1	A	1147	VAL	3.0
1	A	1255	CYS	3.0
1	A	1240	LEU	3.0
1	A	1205	LYS	2.9
1	A	1383	ILE	2.9
1	A	1160	ASP	2.9
1	A	1368	HIS	2.9
1	A	1202	GLY	2.9
1	A	1316	GLY	2.9
1	A	1112	PRO	2.8
1	A	1181	ARG	2.8
1	A	1223	MET	2.8
1	A	1290	MET	2.8
1	A	1264	ARG	2.8
1	A	1154	GLU	2.8
1	A	1107	ASP	2.8
1	A	1159	GLN	2.7
1	A	1332	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1347	ARG	2.7
1	A	1177	GLN	2.7
1	A	1249	ASP	2.7
1	A	1269	GLY	2.6
1	A	1367	GLN	2.6
1	A	1294	LYS	2.6
1	A	1178	ASN	2.6
1	A	1356	GLY	2.5
1	A	1311	ASP	2.5
1	A	1372	ASP	2.5
1	A	1312	THR	2.5
1	A	1354	CYS	2.4
1	A	1299	GLU	2.4
1	A	1375	ASN	2.4
1	A	1331	PRO	2.4
1	A	1104	SER	2.4
1	A	1329	PRO	2.4
1	A	1373	ARG	2.4
1	A	1382	ARG	2.4
1	A	1176	HIS	2.4
1	A	1241	GLU	2.3
1	A	1228	HIS	2.3
1	A	1355	PRO	2.3
1	A	1388	GLN	2.2
1	A	1365	CYS	2.2
1	A	1152	LEU	2.2
1	A	1110	GLU	2.2
1	A	1381	GLU	2.2
1	A	1389	ASP	2.1
1	A	1242	GLU	2.1
1	A	1116	ILE	2.0
1	A	1304	GLY	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 carbohydrates in this entry.

6.4 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. 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, 95^{th} 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(Å^2)	Q<0.9
2	VGH	A	9000	30/30	0.59	0.37	0.99	24,33,42,52	0

6.5 Other polymers

There are no such residues in this entry.