



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:17 AM GMT

PDB ID : 2GHL
Title : Mutant Mus Musculus P38 Kinase Domain in Complex with Inhibitor PG-874743
Authors : Walter, R.L.; Mekel, M.J.; Evdokimov, A.G.; Pokross, M.E.; Brugel, T.A.
Deposited on : 2006-03-27
Resolution : 2.10 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

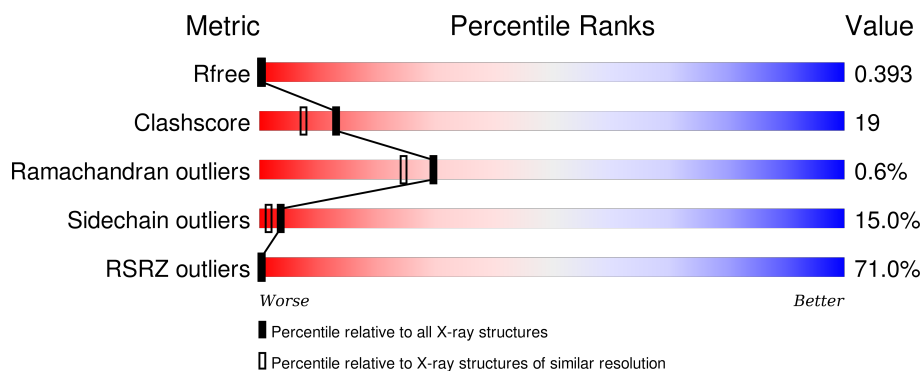
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	348	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3031 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.

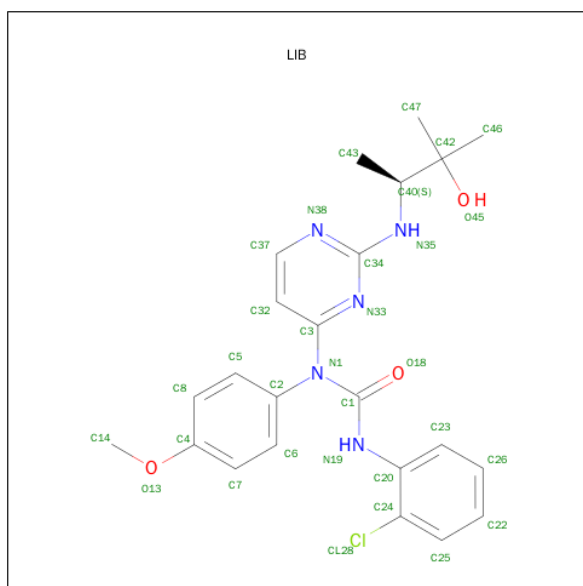
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2689	1726	460	492	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ALA	THR	ENGINEERED	UNP P47811
A	182	PHE	TYR	ENGINEERED	UNP P47811

- Molecule 2 is 3-(2-CHLOROPHENYL)-1-(2-([(1S)-2-HYDROXY-1,2-DIMETHYLPROPYL]AMINO})PYRIMIDIN-4-YL)-1-(4-METHOXYPHENYL)UREA (three-letter code: LIB) (formula: C₂₃H₂₆ClN₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			32	23	1	5	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	310	Total	O	0	0
			310	310		

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 ($\text{RSRZ} > 2$). 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.

- Molecule 1: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.26Å 74.43Å 76.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.45 – 2.10 34.17 – 2.32	Depositor EDS
% Data completeness (in resolution range)	(Not available) (53.45-2.10) 81.0 (34.17-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.199 , 0.301 0.405 , 0.393	Depositor DCC
R_{free} test set	745 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.3	EDS
Estimated twinning fraction	0.020 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 14862 reflections	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	3031	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LIB

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	0.76	2/2752 (0.1%)	0.93	12/3737 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	MET	SD-CE	-6.08	1.43	1.77
1	A	69	TYR	C-N	-5.26	1.22	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	331	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	296	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	321	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	313	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	205	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	124	ASP	CB-CG-OD2	5.62	123.35	118.30
1	A	145	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	227	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	230	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	161	ASP	N-CA-CB	-5.11	101.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ASP	CB-CG-OD2	5.10	122.89	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	LEU	Peptide

5.2 Too-close contacts [i](#)

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	2689	0	2676	101	0
2	A	32	0	26	4	0
3	A	310	0	0	35	0
All	All	3031	0	2702	103	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 19.

All (103) 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:172:ALA:O	1:A:173:ARG:CB	2.18	0.89
1:A:161:ASP:HB3	3:A:666:HOH:O	1.78	0.83
1:A:81:GLU:CD	1:A:81:GLU:H	1.88	0.78
1:A:159:ASN:HB2	3:A:666:HOH:O	1.86	0.75
1:A:111:ALA:HB1	1:A:115:ASN:ND2	2.01	0.75
1:A:149:ARG:NH1	1:A:172:ALA:H	1.85	0.73
1:A:125:ASP:HB3	3:A:641:HOH:O	1.88	0.73
1:A:122:LEU:HD22	3:A:620:HOH:O	1.88	0.73
1:A:167:LEU:HB2	3:A:705:HOH:O	1.88	0.72
1:A:78:MET:HG3	1:A:169:PHE:CE1	2.24	0.72
1:A:166:ILE:O	1:A:169:PHE:HE2	1.73	0.71
1:A:352:PRO:C	3:A:660:HOH:O	2.29	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:HG22	1:A:220:ARG:H	1.57	0.70
1:A:193:ILE:C	1:A:193:ILE:HD13	2.15	0.68
1:A:81:GLU:HG2	3:A:695:HOH:O	1.94	0.67
1:A:60:GLN:HG2	3:A:559:HOH:O	1.95	0.67
1:A:148:HIS:HD2	1:A:150:ASP:H	1.44	0.65
1:A:126:HIS:CD2	3:A:620:HOH:O	2.49	0.65
1:A:166:ILE:HG22	1:A:169:PHE:HD2	1.61	0.65
1:A:116:ILE:HG23	1:A:122:LEU:HD21	1.80	0.64
1:A:87:LEU:HG	1:A:106:THR:HA	1.80	0.64
1:A:149:ARG:NH1	1:A:172:ALA:N	2.46	0.63
1:A:131:ILE:HG21	1:A:213:MET:HE3	1.79	0.63
1:A:139:LYS:NZ	1:A:317:GLU:O	2.29	0.63
1:A:250:ILE:O	1:A:256:ARG:NH1	2.32	0.63
1:A:290:VAL:HG12	3:A:424:HOH:O	1.97	0.63
1:A:152:LYS:HZ2	1:A:185:THR:HG1	1.47	0.63
1:A:78:MET:HG3	1:A:169:PHE:HE1	1.63	0.61
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.84	0.60
1:A:100:ASN:ND2	3:A:634:HOH:O	2.24	0.59
2:A:401:LIB:C26	3:A:635:HOH:O	2.49	0.59
1:A:76:LYS:NZ	1:A:344:GLU:O	2.33	0.59
1:A:172:ALA:HB2	3:A:648:HOH:O	2.01	0.59
1:A:193:ILE:HD13	1:A:194:MET:N	2.18	0.58
1:A:57:ARG:HD3	1:A:60:GLN:NE2	2.19	0.58
1:A:131:ILE:HG13	1:A:213:MET:HE2	1.86	0.57
1:A:214:ALA:O	1:A:218:THR:HB	2.06	0.56
1:A:142:HIS:HD2	3:A:406:HOH:O	1.88	0.56
1:A:171:LEU:N	1:A:172:ALA:O	2.39	0.56
1:A:171:LEU:HD11	1:A:327:PHE:CZ	2.40	0.55
1:A:84:ILE:HD12	1:A:165:LYS:HB3	1.87	0.55
1:A:74:LEU:CD2	1:A:170:GLY:HA3	2.36	0.55
1:A:310:GLN:HG2	3:A:562:HOH:O	2.06	0.54
1:A:155:ASN:CB	3:A:705:HOH:O	2.55	0.54
1:A:249:LYS:NZ	1:A:294:ASP:OD2	2.36	0.54
1:A:83:VAL:HG13	1:A:169:PHE:CE2	2.44	0.53
1:A:184:ALA:HB3	1:A:187:TRP:CE2	2.43	0.53
1:A:290:VAL:O	1:A:296:ARG:HD3	2.09	0.53
1:A:316:ASP:OD1	3:A:661:HOH:O	2.18	0.53
1:A:260:GLN:C	3:A:673:HOH:O	2.46	0.53
1:A:290:VAL:O	1:A:296:ARG:CD	2.57	0.53
1:A:30:VAL:HG12	2:A:401:LIB:CL28	2.46	0.53
1:A:273:VAL:HG23	1:A:274:PHE:CD1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:HIS:CD2	1:A:82:ASN:H	2.28	0.52
1:A:155:ASN:ND2	3:A:705:HOH:O	2.42	0.52
1:A:189:ARG:HD2	3:A:552:HOH:O	2.10	0.52
1:A:27:LEU:HD22	1:A:41:ALA:HB2	1.92	0.52
1:A:124:ASP:OD2	1:A:128:GLN:NE2	2.40	0.51
1:A:81:GLU:OE1	1:A:136:ARG:NH1	2.44	0.50
1:A:74:LEU:HD21	1:A:170:GLY:HA3	1.92	0.50
1:A:287:LYS:CD	3:A:420:HOH:O	2.59	0.50
1:A:280:LEU:CD2	1:A:306:ALA:HB3	2.41	0.50
1:A:253:GLU:O	1:A:257:ASN:HB2	2.12	0.50
1:A:239:VAL:HG21	1:A:291:LEU:HD13	1.94	0.49
1:A:280:LEU:HD21	1:A:306:ALA:HB3	1.94	0.49
1:A:201:ASN:OD1	1:A:203:THR:HG23	2.11	0.49
1:A:35:TYR:HB3	3:A:653:HOH:O	2.12	0.49
1:A:116:ILE:CG2	1:A:122:LEU:HD21	2.43	0.49
1:A:73:ARG:CZ	3:A:703:HOH:O	2.61	0.49
1:A:270:PHE:HA	1:A:273:VAL:HG22	1.95	0.48
1:A:325:GLN:NE2	3:A:707:HOH:O	2.47	0.48
1:A:106:THR:HB	2:A:401:LIB:H142	1.95	0.48
1:A:86:LEU:HD22	1:A:88:ASP:O	2.14	0.47
1:A:218:THR:CG2	1:A:220:ARG:HG3	2.44	0.47
1:A:268:MET:HE2	3:A:702:HOH:O	2.13	0.47
1:A:122:LEU:HD13	3:A:620:HOH:O	2.13	0.47
1:A:269:ASN:ND2	3:A:658:HOH:O	2.47	0.47
1:A:83:VAL:CG1	1:A:169:PHE:CZ	2.98	0.46
1:A:131:ILE:HG21	1:A:213:MET:CE	2.43	0.46
1:A:13:LEU:C	3:A:662:HOH:O	2.55	0.46
1:A:148:HIS:CE1	1:A:169:PHE:HA	2.51	0.45
1:A:218:THR:HG21	3:A:543:HOH:O	2.16	0.45
1:A:142:HIS:HE1	1:A:205:ASP:OD1	2.00	0.45
1:A:189:ARG:HE	1:A:193:ILE:HD11	1.81	0.45
1:A:73:ARG:NH2	3:A:703:HOH:O	2.50	0.45
2:A:401:LIB:N33	2:A:401:LIB:N19	2.59	0.45
1:A:21:PRO:HD3	1:A:90:PHE:CE1	2.53	0.44
1:A:171:LEU:HD12	1:A:328:GLU:OE2	2.18	0.44
1:A:148:HIS:ND1	1:A:169:PHE:HA	2.33	0.43
1:A:193:ILE:C	1:A:193:ILE:CD1	2.83	0.43
1:A:323:TYR:CD2	1:A:325:GLN:HG2	2.55	0.42
1:A:155:ASN:CG	3:A:705:HOH:O	2.57	0.42
1:A:149:ARG:HH12	1:A:172:ALA:N	2.16	0.42
1:A:167:LEU:O	3:A:705:HOH:O	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH2	3:A:653:HOH:O	2.53	0.42
1:A:14:ASN:O	1:A:15:LYS:HB2	2.19	0.41
1:A:155:ASN:HA	1:A:155:ASN:HD22	1.65	0.41
1:A:56:SER:HB3	3:A:692:HOH:O	2.21	0.41
1:A:170:GLY:HA2	1:A:171:LEU:HA	1.83	0.41
1:A:161:ASP:CB	3:A:666:HOH:O	2.53	0.41
1:A:148:HIS:HE1	1:A:167:LEU:O	2.03	0.40
1:A:241:THR:HB	1:A:242:PRO:HD2	2.04	0.40
1:A:129:PHE:O	1:A:133:GLN:HG3	2.21	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	328/348 (94%)	303 (92%)	23 (7%)	2 (1%)	30 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	PHE
1	A	172	ALA

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	293/306 (96%)	249 (85%)	44 (15%)	3 1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	10	ARG
1	A	13	LEU
1	A	17	ILE
1	A	26	ASN
1	A	49	ARG
1	A	60	GLN
1	A	62	ILE
1	A	63	ILE
1	A	64	HIS
1	A	72	LEU
1	A	81	GLU
1	A	86	LEU
1	A	94	ARG
1	A	96	LEU
1	A	100	ASN
1	A	114	ASN
1	A	115	ASN
1	A	117	VAL
1	A	126	HIS
1	A	138	LEU
1	A	169	PHE
1	A	171	LEU
1	A	185	THR
1	A	193	ILE
1	A	194	MET
1	A	198	MET
1	A	218	THR
1	A	220	ARG
1	A	228	HIS
1	A	248	LYS
1	A	252	SER
1	A	254	SER
1	A	256	ARG
1	A	257	ASN
1	A	262	LEU
1	A	264	GLN
1	A	286	GLU

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Mol	Chain	Res	Type
1	A	291	LEU
1	A	295	LYS
1	A	325	GLN
1	A	330	ARG
1	A	333	LEU
1	A	346	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	80	HIS
1	A	107	HIS
1	A	114	ASN
1	A	115	ASN
1	A	142	HIS
1	A	148	HIS
1	A	155	ASN
1	A	257	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](#)

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	LIB	A	401	-	32,34,34	1.08	2 (6%)	43,48,48	2.18	10 (23%)

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	LIB	A	401	-	-	0/28/28/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	LIB	C2-N1	-3.14	1.39	1.44
2	A	401	LIB	C1-N19	-2.57	1.32	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	LIB	N38-C34-N33	-5.73	120.56	126.67
2	A	401	LIB	C32-C3-N33	-4.12	117.22	123.47
2	A	401	LIB	C32-C37-N38	-3.48	119.93	123.90
2	A	401	LIB	C2-N1-C3	-2.07	114.23	118.75
2	A	401	LIB	C34-N33-C3	2.24	121.91	114.23
2	A	401	LIB	N19-C1-N1	3.23	118.88	114.80
2	A	401	LIB	C37-C32-C3	3.29	120.03	116.64
2	A	401	LIB	N35-C34-N33	4.04	122.86	116.95
2	A	401	LIB	C37-N38-C34	5.53	120.29	115.49
2	A	401	LIB	N33-C3-N1	6.14	121.67	114.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	LIB	4	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	334/348 (95%)	3.15	237 (70%) 0 0	28, 47, 70, 79	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	15.8
1	A	35	TYR	13.2
1	A	198	MET	12.2
1	A	185	THR	11.4
1	A	30	VAL	10.7
1	A	197	TRP	9.3
1	A	228	HIS	9.2
1	A	193	ILE	8.6
1	A	232	LEU	8.5
1	A	114	ASN	8.3
1	A	274	PHE	8.0
1	A	199	HIS	7.6
1	A	34	ALA	7.4
1	A	20	VAL	7.4
1	A	170	GLY	7.4
1	A	239	VAL	7.1
1	A	263	ALA	7.0
1	A	117	VAL	6.6
1	A	184	ALA	6.4
1	A	171	LEU	6.3
1	A	14	ASN	6.3
1	A	306	ALA	6.3
1	A	31	GLY	6.2
1	A	275	ILE	6.2
1	A	304	ALA	6.2
1	A	187	TRP	6.0
1	A	200	TYR	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	6.0
1	A	264	GLN	6.0
1	A	129	PHE	5.9
1	A	307	TYR	5.9
1	A	195	LEU	5.8
1	A	259	ILE	5.7
1	A	86	LEU	5.7
1	A	269	ASN	5.5
1	A	276	GLY	5.5
1	A	300	ALA	5.5
1	A	319	VAL	5.3
1	A	258	TYR	5.3
1	A	303	LEU	5.2
1	A	352	PRO	5.2
1	A	113	LEU	5.1
1	A	262	LEU	5.1
1	A	312	HIS	5.1
1	A	11	GLN	5.1
1	A	33	GLY	5.1
1	A	13	LEU	5.1
1	A	131	ILE	4.9
1	A	267	LYS	4.9
1	A	226	THR	4.8
1	A	346	ILE	4.8
1	A	223	PHE	4.8
1	A	311	TYR	4.7
1	A	10	ARG	4.7
1	A	18	TRP	4.7
1	A	126	HIS	4.6
1	A	245	GLU	4.6
1	A	189	ARG	4.6
1	A	164	LEU	4.6
1	A	253	GLU	4.6
1	A	203	THR	4.5
1	A	16	THR	4.5
1	A	74	LEU	4.5
1	A	297	ILE	4.4
1	A	206	ILE	4.4
1	A	310	GLN	4.4
1	A	273	VAL	4.4
1	A	240	GLY	4.3
1	A	103	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	308	PHE	4.2
1	A	27	LEU	4.2
1	A	92	PRO	4.2
1	A	17	ILE	4.1
1	A	173	ARG	4.1
1	A	168	ASP	4.1
1	A	289	LEU	4.1
1	A	255	ALA	4.1
1	A	272	ASN	4.0
1	A	44	THR	4.0
1	A	140	TYR	4.0
1	A	252	SER	4.0
1	A	209	VAL	4.0
1	A	116	ILE	4.0
1	A	106	THR	3.9
1	A	218	THR	3.9
1	A	236	LEU	3.9
1	A	83	VAL	3.9
1	A	43	ASP	3.8
1	A	191	PRO	3.8
1	A	201	ASN	3.8
1	A	62	ILE	3.8
1	A	7	THR	3.8
1	A	214	ALA	3.8
1	A	77	HIS	3.8
1	A	150	ASP	3.7
1	A	32	SER	3.7
1	A	21	PRO	3.7
1	A	48	HIS	3.7
1	A	132	TYR	3.7
1	A	350	PRO	3.6
1	A	225	GLY	3.6
1	A	156	LEU	3.6
1	A	288	MET	3.6
1	A	39	CYS	3.6
1	A	6	PRO	3.6
1	A	8	PHE	3.5
1	A	9	TYR	3.5
1	A	12	GLU	3.5
1	A	158	VAL	3.5
1	A	291	LEU	3.5
1	A	42	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	345	VAL	3.5
1	A	141	ILE	3.5
1	A	280	LEU	3.5
1	A	186	ARG	3.4
1	A	85	GLY	3.4
1	A	102	VAL	3.4
1	A	78	MET	3.4
1	A	318	PRO	3.4
1	A	271	ALA	3.3
1	A	162	CYS	3.3
1	A	81	GLU	3.3
1	A	237	ARG	3.3
1	A	342	TYR	3.3
1	A	50	VAL	3.2
1	A	137	GLY	3.2
1	A	210	GLY	3.2
1	A	340	LEU	3.2
1	A	309	ALA	3.2
1	A	270	PHE	3.2
1	A	213	MET	3.2
1	A	334	ILE	3.1
1	A	87	LEU	3.1
1	A	284	LEU	3.1
1	A	238	LEU	3.1
1	A	128	GLN	3.1
1	A	143	SER	3.1
1	A	122	LEU	3.0
1	A	285	LEU	3.0
1	A	142	HIS	3.0
1	A	144	ALA	3.0
1	A	220	ARG	3.0
1	A	146	ILE	3.0
1	A	90	PHE	3.0
1	A	145	ASP	3.0
1	A	160	GLU	3.0
1	A	216	LEU	3.0
1	A	323	TYR	3.0
1	A	45	LYS	2.9
1	A	234	LEU	2.9
1	A	105	VAL	2.9
1	A	47	GLY	2.9
1	A	204	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	61	SER	2.9
1	A	294	ASP	2.9
1	A	130	LEU	2.9
1	A	295	LYS	2.8
1	A	133	GLN	2.8
1	A	268	MET	2.8
1	A	19	GLU	2.8
1	A	188	TYR	2.8
1	A	115	ASN	2.8
1	A	283	ASP	2.8
1	A	63	ILE	2.8
1	A	147	ILE	2.8
1	A	327	PHE	2.7
1	A	266	PRO	2.7
1	A	329	SER	2.7
1	A	265	MET	2.7
1	A	163	GLU	2.7
1	A	26	ASN	2.7
1	A	127	VAL	2.7
1	A	157	ALA	2.7
1	A	5	ARG	2.6
1	A	155	ASN	2.6
1	A	317	GLU	2.6
1	A	166	ILE	2.6
1	A	153	PRO	2.6
1	A	167	LEU	2.6
1	A	293	SER	2.6
1	A	101	ASP	2.6
1	A	75	LEU	2.6
1	A	104	LEU	2.6
1	A	194	MET	2.6
1	A	250	ILE	2.6
1	A	349	VAL	2.6
1	A	46	THR	2.5
1	A	134	ILE	2.5
1	A	108	LEU	2.5
1	A	59	PHE	2.5
1	A	97	GLU	2.5
1	A	290	VAL	2.5
1	A	332	LEU	2.4
1	A	212	ILE	2.4
1	A	343	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	219	GLY	2.4
1	A	95	SER	2.4
1	A	254	SER	2.4
1	A	28	SER	2.4
1	A	56	SER	2.4
1	A	38	VAL	2.4
1	A	151	LEU	2.4
1	A	260	GLN	2.4
1	A	91	THR	2.3
1	A	135	LEU	2.3
1	A	161	ASP	2.3
1	A	24	TYR	2.3
1	A	305	HIS	2.3
1	A	278	ASN	2.3
1	A	154	SER	2.2
1	A	227	ASP	2.2
1	A	229	ILE	2.2
1	A	37	SER	2.2
1	A	208	SER	2.2
1	A	222	LEU	2.2
1	A	326	SER	2.2
1	A	233	LYS	2.2
1	A	341	THR	2.2
1	A	110	GLY	2.2
1	A	190	ALA	2.2
1	A	72	LEU	2.2
1	A	330	ARG	2.2
1	A	99	PHE	2.2
1	A	125	ASP	2.2
1	A	299	ALA	2.2
1	A	51	ALA	2.1
1	A	93	ALA	2.1
1	A	321	ASP	2.1
1	A	123	THR	2.1
1	A	211	CYS	2.1
1	A	53	LYS	2.1
1	A	25	GLN	2.1
1	A	94	ARG	2.1
1	A	251	SER	2.1
1	A	111	ALA	2.1
1	A	281	ALA	2.1
1	A	257	ASN	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 [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	LIB	A	401	32/32	0.74	0.27	-0.28	30,38,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.