



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:22 AM GMT

PDB ID : 2GTN
Title : Mutated MAP kinase P38 (Mus Musculus) in complex with Inhibitor PG-951717
Authors : Walter, R.L.; Mekel, M.J.; Evdokimov, A.G.; Pokross, M.E.; Sabat, M.
Deposited on : 2006-04-28
Resolution : 1.80 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

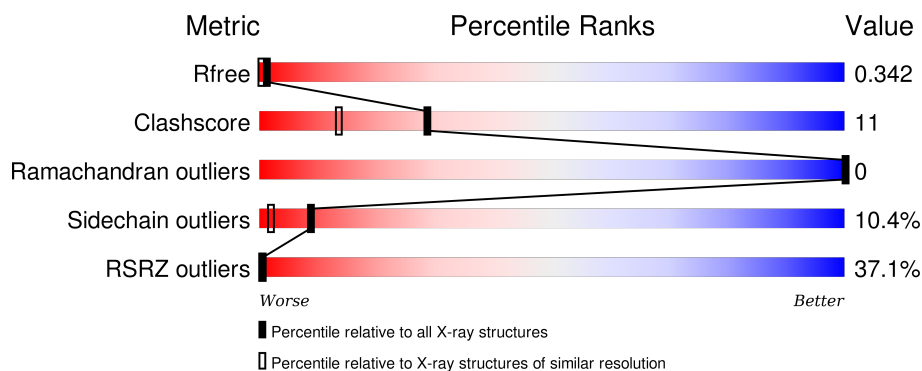
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	353	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2972 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.

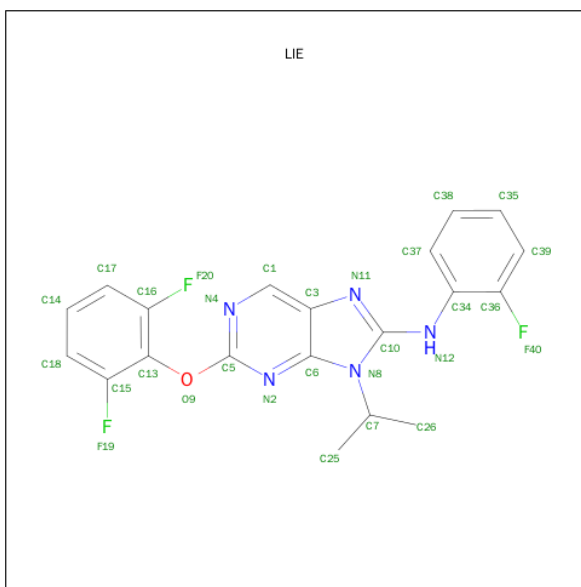
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2717	1743	466	496	12			

- 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 2-(2,6-DIFLUOROPHENOXY)-N-(2-FLUOROPHENYL)-9-ISOPROPYL-9H-PURIN-8-AMINE (three-letter code: LIE) (formula: C₂₀H₁₆F₃N₅O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			29	20	3	5	1		

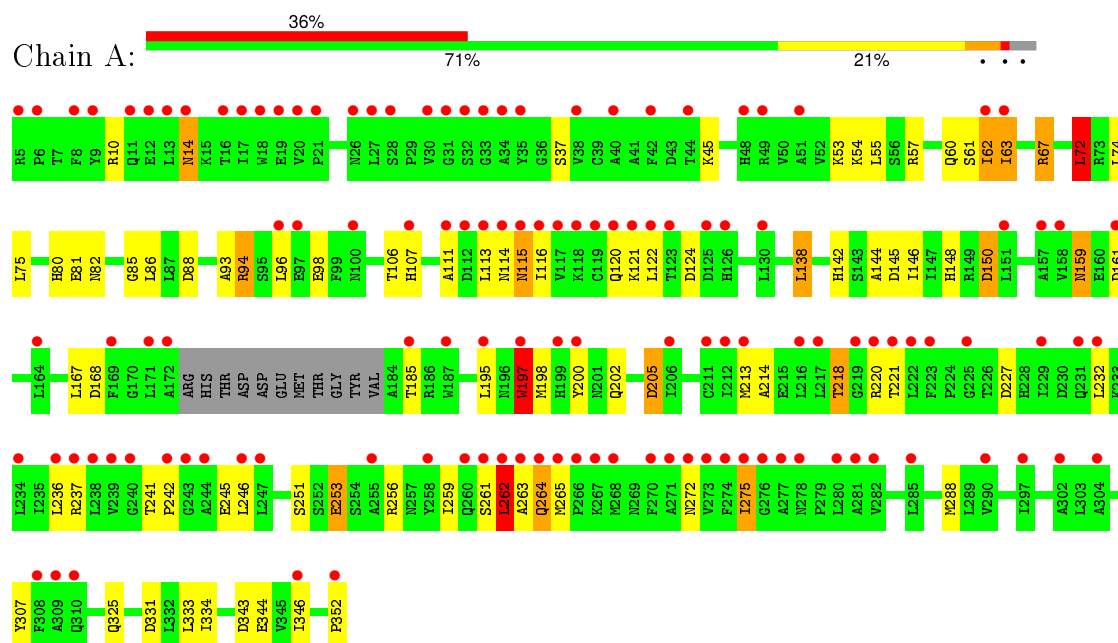
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	221	Total	O	0	0
			221	221		

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	64.99Å 74.55Å 78.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 41.49 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.8 (50.00-1.80) 95.3 (41.49-1.82)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.248 0.319 , 0.342	Depositor DCC
R_{free} test set	1678 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.3	EDS
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 33303 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2972	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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: LIE, SO4

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	0.87	3/2781 (0.1%)	0.98	12/3775 (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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	262	LEU	N-CA	-7.82	1.30	1.46
1	A	288	MET	SD-CE	-5.52	1.47	1.77
1	A	197	TRP	CB-CG	5.13	1.59	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ASP	CB-CG-OD2	10.81	128.03	118.30
1	A	262	LEU	N-CA-C	-8.93	86.90	111.00
1	A	88	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	331	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	124	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	227	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	205	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	150	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	343	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	67	ARG	NE-CZ-NH1	5.15	122.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	LEU	CB-CG-CD2	5.08	119.64	111.00
1	A	138	LEU	CB-CG-CD1	5.03	119.56	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	263	ALA	Peptide

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	2717	0	2715	61	0
2	A	5	0	0	1	0
3	A	29	0	16	2	0
4	A	221	0	0	23	0
All	All	2972	0	2731	63	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 (63) 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:111:ALA:HB1	1:A:115:ASN:HD21	1.03	1.18
1:A:111:ALA:HB1	1:A:115:ASN:ND2	1.87	0.89
1:A:80:HIS:HD2	1:A:82:ASN:H	1.21	0.88
1:A:53:LYS:HG2	4:A:556:HOH:O	1.74	0.86
1:A:107:HIS:ND1	2:A:353:SO4:O4	2.13	0.80
1:A:81:GLU:HG2	4:A:396:HOH:O	1.84	0.77
1:A:98:GLU:HB2	4:A:507:HOH:O	1.85	0.77
1:A:63:ILE:HD11	1:A:67:ARG:NH2	2.03	0.74
1:A:75:LEU:HB3	1:A:86:LEU:HG	1.73	0.70
1:A:218:THR:HG22	1:A:220:ARG:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASN:C	1:A:115:ASN:HD22	1.95	0.69
1:A:272:ASN:O	1:A:275:ILE:HG12	1.92	0.69
1:A:218:THR:HG21	4:A:377:HOH:O	1.92	0.69
3:A:354:LIE:H35	4:A:565:HOH:O	1.94	0.67
1:A:86:LEU:HD23	4:A:565:HOH:O	1.94	0.67
1:A:148:HIS:HD2	1:A:150:ASP:H	1.42	0.67
1:A:57:ARG:HD2	1:A:60:GLN:HE22	1.60	0.66
1:A:242:PRO:HB3	1:A:246:LEU:HD23	1.77	0.66
1:A:261:SER:C	1:A:262:LEU:O	2.29	0.64
1:A:81:GLU:CG	4:A:396:HOH:O	2.43	0.64
1:A:55:LEU:HD23	4:A:556:HOH:O	1.97	0.63
1:A:55:LEU:HA	4:A:556:HOH:O	1.98	0.62
1:A:106:THR:HG23	4:A:565:HOH:O	2.00	0.62
1:A:197:TRP:HD1	1:A:200:TYR:CE1	2.18	0.61
1:A:80:HIS:CD2	1:A:82:ASN:H	2.11	0.60
1:A:94:ARG:HG2	4:A:575:HOH:O	2.01	0.60
1:A:214:ALA:O	1:A:218:THR:HB	2.00	0.60
1:A:115:ASN:ND2	1:A:115:ASN:O	2.33	0.60
1:A:148:HIS:HE1	1:A:167:LEU:O	1.85	0.58
1:A:352:PRO:O	4:A:523:HOH:O	2.17	0.58
1:A:142:HIS:HD2	4:A:360:HOH:O	1.87	0.56
1:A:159:ASN:C	1:A:159:ASN:HD22	2.09	0.56
1:A:218:THR:CG2	1:A:220:ARG:H	2.20	0.55
1:A:57:ARG:HD2	1:A:60:GLN:NE2	2.23	0.54
1:A:325:GLN:NE2	4:A:438:HOH:O	2.40	0.53
1:A:93:ALA:HA	4:A:507:HOH:O	2.11	0.50
1:A:232:LEU:HD21	1:A:259:ILE:HG12	1.94	0.50
1:A:144:ALA:HB3	1:A:146:ILE:HD12	1.92	0.50
1:A:145:ASP:OD1	4:A:554:HOH:O	2.20	0.50
1:A:80:HIS:HE1	4:A:363:HOH:O	1.94	0.50
1:A:85:GLY:O	1:A:106:THR:HG22	2.12	0.50
1:A:14:ASN:OD1	1:A:14:ASN:N	2.45	0.50
1:A:142:HIS:HE1	1:A:205:ASP:OD1	1.94	0.50
1:A:344:GLU:C	4:A:569:HOH:O	2.50	0.49
1:A:236:LEU:HD12	1:A:262:LEU:HD13	1.93	0.49
1:A:197:TRP:HD1	1:A:200:TYR:CZ	2.30	0.49
1:A:264:GLN:HG3	1:A:265:MET:N	2.28	0.48
1:A:237:ARG:HD2	4:A:548:HOH:O	2.13	0.48
1:A:72:LEU:HD11	4:A:569:HOH:O	2.14	0.48
1:A:61:SER:HA	1:A:334:ILE:HD11	1.97	0.47
1:A:62:ILE:HG22	1:A:334:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:PRO:HG3	1:A:259:ILE:HG21	1.98	0.46
1:A:253:GLU:CD	1:A:256:ARG:HH22	2.19	0.45
1:A:198:MET:SD	1:A:251:SER:OG	2.74	0.44
1:A:272:ASN:O	1:A:275:ILE:CG1	2.66	0.43
1:A:150:ASP:OD2	1:A:185:THR:HG23	2.17	0.43
1:A:253:GLU:HG2	1:A:253:GLU:H	1.64	0.43
1:A:116:ILE:O	1:A:116:ILE:CG2	2.67	0.43
1:A:213:MET:HE1	1:A:307:TYR:CE2	2.53	0.43
1:A:202:GLN:NE2	4:A:554:HOH:O	2.51	0.42
1:A:94:ARG:HB3	1:A:94:ARG:CZ	2.49	0.42
1:A:54:LYS:C	4:A:556:HOH:O	2.57	0.42
3:A:354:LIE:C35	4:A:565:HOH:O	2.60	0.41

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	333/348 (96%)	324 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	297/307 (97%)	266 (90%)	31 (10%)	9 2

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	14	ASN
1	A	37	SER
1	A	45	LYS
1	A	62	ILE
1	A	63	ILE
1	A	72	LEU
1	A	74	LEU
1	A	94	ARG
1	A	96	LEU
1	A	113	LEU
1	A	114	ASN
1	A	115	ASN
1	A	120	GLN
1	A	121	LYS
1	A	122	LEU
1	A	138	LEU
1	A	159	ASN
1	A	161	ASP
1	A	195	LEU
1	A	197	TRP
1	A	218	THR
1	A	221	THR
1	A	241	THR
1	A	245	GLU
1	A	253	GLU
1	A	262	LEU
1	A	264	GLN
1	A	275	ILE
1	A	333	LEU
1	A	346	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	60	GLN

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Mol	Chain	Res	Type
1	A	64	HIS
1	A	80	HIS
1	A	114	ASN
1	A	115	ASN
1	A	120	GLN
1	A	142	HIS
1	A	148	HIS
1	A	159	ASN
1	A	228	HIS
1	A	257	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 ⓘ

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	$\# Z > 2$
2	SO4	A	353	-	4,4,4	0.58	0	6,6,6	0.76	0
3	LIE	A	354	-	28,32,32	1.07	2 (7%)	35,46,46	2.25	9 (25%)

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	SO4	A	353	-	-	0/0/0/0	0/0/0/0
3	LIE	A	354	-	-	0/10/12/12	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	354	LIE	C1-N4	2.22	1.35	1.32
3	A	354	LIE	C5-N4	2.96	1.36	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	354	LIE	N4-C5-N2	-7.88	123.31	128.33
3	A	354	LIE	C10-N11-C3	-5.16	99.36	106.64
3	A	354	LIE	C34-N12-C10	-4.08	120.34	128.84
3	A	354	LIE	C39-C36-C34	-2.32	120.88	123.36
3	A	354	LIE	C1-N4-C5	2.13	117.42	115.06
3	A	354	LIE	F19-C15-C18	2.52	124.19	118.47
3	A	354	LIE	C3-C6-N8	2.69	111.14	106.15
3	A	354	LIE	F40-C36-C34	2.92	120.43	117.50
3	A	354	LIE	C37-C34-C36	4.17	121.21	117.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	353	SO4	1	0
3	A	354	LIE	2	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, 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	337/348 (96%)	1.84	125 (37%) 0 0	19, 33, 53, 77	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	6.6
1	A	262	LEU	6.4
1	A	263	ALA	6.1
1	A	116	ILE	6.0
1	A	271	ALA	5.4
1	A	35	TYR	5.4
1	A	120	GLN	5.3
1	A	17	ILE	5.2
1	A	219	GLY	5.2
1	A	117	VAL	5.2
1	A	119	CYS	5.1
1	A	115	ASN	5.0
1	A	276	GLY	4.9
1	A	268	MET	4.8
1	A	16	THR	4.8
1	A	197	TRP	4.7
1	A	274	PHE	4.6
1	A	33	GLY	4.6
1	A	14	ASN	4.2
1	A	239	VAL	4.1
1	A	122	LEU	4.1
1	A	266	PRO	4.1
1	A	9	TYR	4.0
1	A	13	LEU	4.0
1	A	232	LEU	4.0
1	A	225	GLY	3.9
1	A	273	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	123	THR	3.9
1	A	118	LYS	3.8
1	A	280	LEU	3.8
1	A	275	ILE	3.8
1	A	270	PHE	3.7
1	A	34	ALA	3.7
1	A	261	SER	3.7
1	A	42	PHE	3.7
1	A	229	ILE	3.6
1	A	267	LYS	3.6
1	A	169	PHE	3.6
1	A	223	PHE	3.6
1	A	28	SER	3.5
1	A	217	LEU	3.5
1	A	195	LEU	3.5
1	A	121	LYS	3.4
1	A	290	VAL	3.4
1	A	113	LEU	3.3
1	A	18	TRP	3.3
1	A	21	PRO	3.2
1	A	31	GLY	3.2
1	A	30	VAL	3.2
1	A	100	ASN	3.2
1	A	277	ALA	3.2
1	A	211	CYS	3.2
1	A	236	LEU	3.2
1	A	247	LEU	3.1
1	A	111	ALA	3.1
1	A	238	LEU	3.1
1	A	265	MET	3.1
1	A	107	HIS	3.0
1	A	221	THR	3.0
1	A	272	ASN	3.0
1	A	51	ALA	3.0
1	A	258	TYR	2.9
1	A	352	PRO	2.9
1	A	40	ALA	2.9
1	A	255	ALA	2.9
1	A	304	ALA	2.9
1	A	20	VAL	2.9
1	A	243	GLY	2.8
1	A	32	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	158	VAL	2.8
1	A	246	LEU	2.8
1	A	285	LEU	2.8
1	A	281	ALA	2.8
1	A	308	PHE	2.8
1	A	49	ARG	2.7
1	A	8	PHE	2.7
1	A	213	MET	2.6
1	A	242	PRO	2.6
1	A	114	ASN	2.6
1	A	220	ARG	2.6
1	A	125	ASP	2.5
1	A	157	ALA	2.5
1	A	282	VAL	2.4
1	A	206	ILE	2.4
1	A	26	ASN	2.4
1	A	199	HIS	2.4
1	A	11	GLN	2.4
1	A	264	GLN	2.4
1	A	96	LEU	2.4
1	A	151	LEU	2.4
1	A	38	VAL	2.4
1	A	6	PRO	2.4
1	A	27	LEU	2.4
1	A	200	TYR	2.4
1	A	48	HIS	2.4
1	A	97	GLU	2.3
1	A	302	ALA	2.3
1	A	63	ILE	2.3
1	A	164	LEU	2.3
1	A	216	LEU	2.3
1	A	231	GLN	2.3
1	A	244	ALA	2.3
1	A	130	LEU	2.3
1	A	222	LEU	2.3
1	A	5	ARG	2.2
1	A	171	LEU	2.2
1	A	234	LEU	2.2
1	A	187	TRP	2.2
1	A	260	GLN	2.2
1	A	346	ILE	2.2
1	A	240	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	297	ILE	2.2
1	A	12	GLU	2.1
1	A	112	ASP	2.1
1	A	212	ILE	2.1
1	A	44	THR	2.1
1	A	19	GLU	2.1
1	A	310	GLN	2.1
1	A	237	ARG	2.0
1	A	185	THR	2.0
1	A	309	ALA	2.0
1	A	126	HIS	2.0
1	A	161	ASP	2.0
1	A	278	ASN	2.0
1	A	62	ILE	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(Å ²)	Q<0.9
2	SO4	A	353	5/5	0.83	0.30	2.85	45,47,49,52	0
3	LIE	A	354	29/29	0.84	0.15	-0.75	21,26,33,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.