



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:06 PM GMT

PDB ID : 3VUL
Title : Crystal structure of a cysteine-deficient mutant M1 in MAP kinase JNK1
Authors : Nakaniwa, T.; Kinoshita, T.; Inoue, T.
Deposited on : 2012-07-02
Resolution : 2.81 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

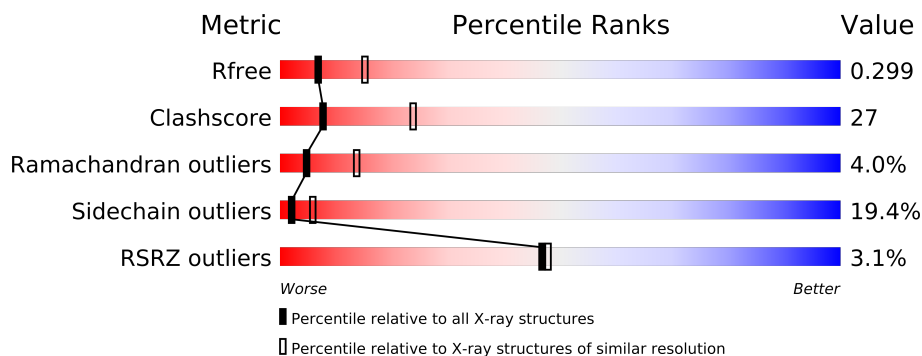
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.81 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}	66092	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	370	
2	F	11	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2896 atoms, of which 0 are hydrogen and 0 are deuterium.

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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2775	1782	469	511	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	VAL	CYS	ENGINEERED MUTATION	UNP A1L4K2
A	116	SER	CYS	ENGINEERED MUTATION	UNP A1L4K2
A	137	VAL	CYS	ENGINEERED MUTATION	UNP A1L4K2
A	163	ALA	CYS	ENGINEERED MUTATION	UNP A1L4K2
A	213	VAL	CYS	ENGINEERED MUTATION	UNP A1L4K2
A	245	SER	CYS	ENGINEERED MUTATION	UNP A1L4K2
A	365	HIS	-	EXPRESSION TAG	UNP A1L4K2
A	366	HIS	-	EXPRESSION TAG	UNP A1L4K2
A	367	HIS	-	EXPRESSION TAG	UNP A1L4K2
A	368	HIS	-	EXPRESSION TAG	UNP A1L4K2
A	369	HIS	-	EXPRESSION TAG	UNP A1L4K2
A	370	HIS	-	EXPRESSION TAG	UNP A1L4K2

- Molecule 2 is a protein called Peptide from C-Jun-amino-terminal kinase-interacting protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	0	0	0
			84	55	15	14			

- Molecule 3 is water.

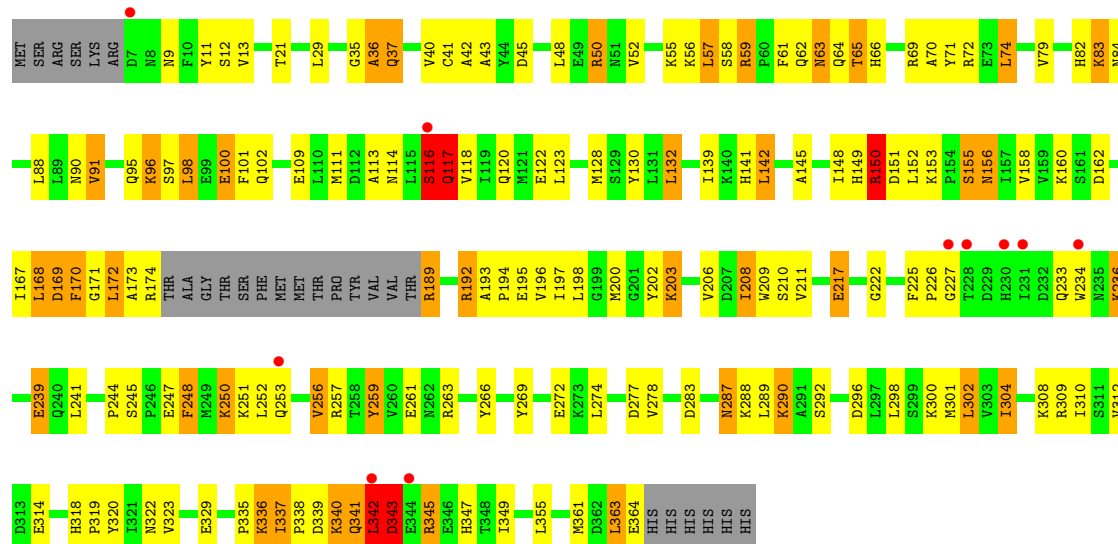
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	36	Total	O	0	0
			36	36		
3	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

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: Mitogen-activated protein kinase 8

Chain A: 



- Molecule 2: Peptide from C-Jun-amino-terminal kinase-interacting protein 1

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	161.78Å 161.78Å 87.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.78 – 2.81 33.78 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.6 (33.78-2.81) 98.5 (33.78-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.249 , 0.315 0.242 , 0.299	Depositor DCC
R_{free} test set	853 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	55.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 16807 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2896	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.80	2/2836 (0.1%)	0.89	2/3837 (0.1%)
2	F	1.20	0/86	1.10	0/114
All	All	0.81	2/2922 (0.1%)	0.90	2/3951 (0.1%)

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	41	CYS	CB-SG	-6.29	1.71	1.82
1	A	239	GLU	CG-CD	5.02	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	SER	C-N-CA	5.20	134.71	121.70
1	A	168	LEU	CA-CB-CG	5.16	127.17	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2775	0	2790	156	0
2	F	84	0	91	4	0
3	A	36	0	0	4	0
3	F	1	0	0	0	0
All	All	2896	0	2881	157	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 27.

All (157) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:HIS:HD2	1:A:84:ASN:H	1.07	0.99
1:A:304:ILE:H	1:A:304:ILE:HD12	1.28	0.99
1:A:170:PHE:HA	1:A:173:ALA:HB3	1.55	0.89
1:A:56:LYS:HE2	1:A:58:SER:OG	1.75	0.85
1:A:233:GLN:HG3	1:A:234:TRP:H	1.39	0.85
1:A:29:LEU:HD22	1:A:43:ALA:HB2	1.56	0.85
1:A:116:SER:N	1:A:117:GLN:HB2	1.91	0.84
1:A:40:VAL:HG22	1:A:55:LYS:HB2	1.57	0.84
1:A:82:HIS:CD2	1:A:84:ASN:H	1.95	0.84
1:A:318:HIS:HD2	1:A:320:TYR:H	1.24	0.82
1:A:337:ILE:HG22	1:A:338:PRO:HD2	1.66	0.77
1:A:343:ASP:HA	3:A:419:HOH:O	1.86	0.76
1:A:36:ALA:HB3	1:A:37:GLN:HE21	1.51	0.75
1:A:239:GLU:HB3	3:A:431:HOH:O	1.85	0.75
1:A:318:HIS:CD2	1:A:320:TYR:H	2.04	0.74
1:A:82:HIS:HD2	1:A:84:ASN:N	1.85	0.71
1:A:208:ILE:HG22	1:A:309:ARG:HD3	1.72	0.71
1:A:233:GLN:HG3	1:A:234:TRP:N	2.05	0.70
1:A:111:MET:HE3	1:A:160:LYS:HB2	1.74	0.69
1:A:149:HIS:HD2	1:A:151:ASP:H	1.42	0.68
1:A:37:GLN:NE2	1:A:37:GLN:H	1.92	0.67
1:A:170:PHE:C	1:A:172:LEU:H	1.97	0.67
1:A:169:ASP:O	1:A:170:PHE:CD1	2.47	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:TYR:HE1	1:A:263:ARG:HD3	1.60	0.66
1:A:141:HIS:CE1	1:A:335:PRO:HD3	2.30	0.66
1:A:194:PRO:HA	1:A:197:ILE:HG12	1.77	0.66
1:A:203:LYS:O	1:A:206:VAL:HG12	1.96	0.66
2:F:555:LYS:HD2	2:F:556:ARG:H	1.61	0.64
1:A:290:LYS:NZ	1:A:292:SER:HB3	2.13	0.63
1:A:170:PHE:HA	1:A:173:ALA:CB	2.27	0.63
1:A:304:ILE:H	1:A:304:ILE:CD1	1.91	0.63
1:A:338:PRO:C	1:A:340:LYS:H	2.02	0.63
1:A:169:ASP:HB3	1:A:172:LEU:HD21	1.80	0.62
1:A:341:GLN:HE22	1:A:343:ASP:H	1.48	0.62
1:A:195:GLU:HA	1:A:200:MET:HE3	1.81	0.62
1:A:111:MET:CE	1:A:160:LYS:HB2	2.29	0.61
1:A:250:LYS:HE2	1:A:257:ARG:NH1	2.16	0.61
1:A:98:LEU:HD12	1:A:98:LEU:O	2.01	0.60
1:A:59:ARG:NH1	1:A:102:GLN:OE1	2.34	0.60
1:A:156:ASN:HD22	1:A:156:ASN:C	2.05	0.60
1:A:338:PRO:O	1:A:340:LYS:N	2.30	0.59
1:A:170:PHE:CA	1:A:173:ALA:HB3	2.30	0.59
1:A:153:LYS:H	1:A:156:ASN:HD21	1.49	0.59
1:A:189:ARG:HA	1:A:192:ARG:HH21	1.66	0.59
1:A:288:LYS:HD2	1:A:323:VAL:HG12	1.85	0.57
1:A:128:MET:O	1:A:132:LEU:HD22	2.04	0.57
1:A:244:PRO:HB2	1:A:248:PHE:CD2	2.40	0.57
1:A:211:VAL:HG12	1:A:301:MET:HE3	1.87	0.57
1:A:114:ASN:HD22	1:A:155:SER:HA	1.70	0.56
1:A:148:ILE:H	1:A:174:ARG:C	2.09	0.56
1:A:162:ASP:HA	2:F:558:THR:O	2.06	0.56
1:A:300:LYS:O	1:A:310:ILE:HG22	2.04	0.56
1:A:116:SER:CA	1:A:117:GLN:HB2	2.35	0.56
1:A:250:LYS:O	1:A:252:LEU:N	2.39	0.56
1:A:95:GLN:HB3	1:A:100:GLU:HG2	1.88	0.55
1:A:208:ILE:HG23	1:A:301:MET:CG	2.36	0.55
1:A:170:PHE:HB3	1:A:173:ALA:HB3	1.89	0.54
1:A:208:ILE:HD11	1:A:312:VAL:HA	1.88	0.54
1:A:329:GLU:OE2	2:F:556:ARG:NH1	2.35	0.54
1:A:29:LEU:HD22	1:A:43:ALA:CB	2.32	0.54
1:A:145:ALA:CB	1:A:335:PRO:HG2	2.39	0.53
1:A:114:ASN:ND2	1:A:155:SER:HA	2.21	0.53
1:A:283:ASP:CG	1:A:290:LYS:HG2	2.29	0.53
1:A:290:LYS:HZ3	1:A:292:SER:HB3	1.74	0.52
1:A:211:VAL:HG12	1:A:301:MET:CE	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139:ILE:HD11	1:A:152:LEU:CD1	2.39	0.52
1:A:225:PHE:O	1:A:227:GLY:N	2.44	0.51
1:A:259:TYR:CD1	1:A:259:TYR:C	2.83	0.51
1:A:338:PRO:HB2	1:A:340:LYS:HB3	1.93	0.51
1:A:59:ARG:HH11	1:A:102:GLN:HB3	1.76	0.50
1:A:96:LYS:HD2	1:A:100:GLU:OE1	2.12	0.50
1:A:341:GLN:HE22	1:A:343:ASP:N	2.08	0.50
1:A:338:PRO:C	1:A:340:LYS:N	2.64	0.50
1:A:340:LYS:NZ	1:A:341:GLN:HB2	2.26	0.50
1:A:193:ALA:HB3	1:A:206:VAL:HG23	1.93	0.50
1:A:217:GLU:HG3	1:A:222:GLY:O	2.11	0.50
1:A:59:ARG:NH2	3:A:436:HOH:O	2.25	0.49
1:A:345:ARG:HD2	3:A:419:HOH:O	2.12	0.49
1:A:64:GLN:NE2	1:A:347:HIS:O	2.46	0.49
1:A:208:ILE:HG23	1:A:301:MET:HG3	1.94	0.49
1:A:59:ARG:HH11	1:A:102:GLN:CB	2.24	0.49
1:A:63:ASN:HD22	1:A:66:HIS:CD2	2.31	0.48
1:A:310:ILE:HG13	1:A:314:GLU:HB2	1.95	0.48
1:A:304:ILE:HD12	1:A:304:ILE:N	2.12	0.48
1:A:202:TYR:O	1:A:203:LYS:HD2	2.13	0.48
1:A:63:ASN:HD21	1:A:65:THR:HB	1.79	0.48
1:A:239:GLU:HG3	1:A:266:TYR:CZ	2.49	0.48
1:A:63:ASN:ND2	1:A:66:HIS:CD2	2.82	0.47
1:A:208:ILE:HG23	1:A:301:MET:HG2	1.97	0.47
1:A:151:ASP:CG	1:A:151:ASP:O	2.53	0.47
1:A:63:ASN:ND2	1:A:66:HIS:HD2	2.13	0.47
1:A:83:LYS:HE3	1:A:329:GLU:HG2	1.96	0.47
1:A:70:ALA:O	1:A:74:LEU:HD22	2.15	0.47
1:A:336:LYS:HG3	1:A:336:LYS:O	2.14	0.47
1:A:37:GLN:HE21	1:A:37:GLN:H	1.63	0.47
1:A:361:MET:CE	1:A:361:MET:HA	2.45	0.47
1:A:170:PHE:CB	1:A:173:ALA:HB3	2.45	0.47
1:A:141:HIS:NE2	1:A:335:PRO:HD3	2.30	0.46
1:A:310:ILE:HG21	1:A:310:ILE:HD13	1.66	0.46
1:A:247:GLU:O	1:A:247:GLU:HG2	2.14	0.46
1:A:168:LEU:O	1:A:169:ASP:HB2	2.15	0.46
1:A:259:TYR:HE1	1:A:263:ARG:CD	2.26	0.46
1:A:195:GLU:HA	1:A:200:MET:CE	2.45	0.46
1:A:59:ARG:NH1	1:A:102:GLN:HB3	2.31	0.46
1:A:160:LYS:HB3	1:A:162:ASP:OD1	2.15	0.46
1:A:225:PHE:HA	1:A:236:LYS:HD2	1.97	0.46
1:A:277:ASP:O	1:A:278:VAL:C	2.54	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:ILE:CG2	1:A:338:PRO:HD2	2.40	0.45
1:A:193:ALA:O	1:A:196:VAL:HB	2.17	0.45
1:A:253:GLN:HB2	1:A:256:VAL:HB	1.99	0.45
1:A:83:LYS:HE3	1:A:329:GLU:CG	2.46	0.45
1:A:170:PHE:C	1:A:172:LEU:N	2.67	0.45
1:A:72:ARG:HD3	1:A:173:ALA:O	2.17	0.45
1:A:145:ALA:HB3	1:A:335:PRO:HG2	1.99	0.45
1:A:296:ASP:OD2	1:A:318:HIS:HE1	2.00	0.44
1:A:361:MET:HE3	1:A:361:MET:HA	1.99	0.44
1:A:11:TYR:O	1:A:21:THR:HA	2.17	0.44
1:A:113:ALA:HB1	1:A:117:GLN:OE1	2.17	0.44
1:A:250:LYS:HE2	1:A:257:ARG:HH12	1.82	0.44
1:A:150:ARG:NH1	1:A:172:LEU:O	2.46	0.44
1:A:150:ARG:HB2	1:A:150:ARG:CZ	2.47	0.44
1:A:111:MET:HG3	1:A:158:VAL:CG2	2.48	0.44
1:A:97:SER:O	1:A:101:PHE:N	2.51	0.44
1:A:139:ILE:HD11	1:A:152:LEU:HD13	2.00	0.44
1:A:342:LEU:O	1:A:343:ASP:C	2.57	0.44
1:A:167:ILE:HG22	1:A:168:LEU:O	2.18	0.43
1:A:150:ARG:NH1	1:A:174:ARG:HG2	2.33	0.43
1:A:61:PHE:HE2	1:A:102:GLN:HA	1.83	0.43
1:A:63:ASN:OD1	1:A:64:GLN:N	2.51	0.43
1:A:71:TYR:CE2	1:A:341:GLN:HG2	2.54	0.43
1:A:59:ARG:HA	1:A:102:GLN:O	2.19	0.43
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.80	0.43
1:A:241:LEU:HD11	1:A:302:LEU:HD22	2.01	0.42
1:A:45:ASP:C	1:A:45:ASP:OD1	2.57	0.42
1:A:91:VAL:HG22	1:A:363:LEU:HB3	2.01	0.42
1:A:318:HIS:CD2	1:A:319:PRO:HD2	2.54	0.42
1:A:153:LYS:H	1:A:156:ASN:ND2	2.16	0.42
1:A:50:ARG:HD3	1:A:52:VAL:HG12	2.00	0.42
1:A:197:ILE:HG13	1:A:198:LEU:HG	2.01	0.42
1:A:130:TYR:CD2	2:F:557:PRO:HD2	2.54	0.42
1:A:193:ALA:HB1	1:A:195:GLU:OE1	2.20	0.41
1:A:257:ARG:NH1	1:A:261:GLU:OE2	2.53	0.41
1:A:88:LEU:HD11	1:A:91:VAL:HG12	2.02	0.41
1:A:345:ARG:HD3	1:A:347:HIS:NE2	2.35	0.41
1:A:37:GLN:O	1:A:57:LEU:HD23	2.21	0.41
1:A:198:LEU:HD12	1:A:200:MET:CE	2.50	0.41
1:A:209:TRP:O	1:A:210:SER:C	2.58	0.41
1:A:150:ARG:HH11	1:A:174:ARG:HG2	1.85	0.41
1:A:283:ASP:OD1	1:A:290:LYS:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:LEU:HD22	1:A:256:VAL:CG1	2.51	0.41
1:A:269:TYR:HB2	1:A:274:LEU:HG	2.02	0.41
1:A:29:LEU:HA	1:A:42:ALA:O	2.21	0.41
1:A:35:GLY:O	1:A:37:GLN:N	2.54	0.41
1:A:118:VAL:HG13	1:A:123:LEU:HD11	2.02	0.41
1:A:151:ASP:OD2	1:A:172:LEU:HG	2.21	0.40
1:A:290:LYS:HZ3	1:A:292:SER:CB	2.34	0.40
1:A:252:LEU:HB3	1:A:256:VAL:HG12	2.03	0.40

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	340/370 (92%)	294 (86%)	32 (9%)	14 (4%)	4	13
2	F	8/11 (73%)	8 (100%)	0	0	100	100
All	All	348/381 (91%)	302 (87%)	32 (9%)	14 (4%)	5	14

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ALA
1	A	117	GLN
1	A	339	ASP
1	A	343	ASP
1	A	251	LYS
1	A	65	THR
1	A	226	PRO
1	A	342	LEU
1	A	169	ASP
1	A	287	ASN
1	A	349	ILE
1	A	9	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	ARG
1	A	171	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	305/331 (92%)	246 (81%)	59 (19%)	2	6
2	F	10/11 (91%)	8 (80%)	2 (20%)	2	5
All	All	315/342 (92%)	254 (81%)	61 (19%)	2	6

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	13	VAL
1	A	37	GLN
1	A	48	LEU
1	A	50	ARG
1	A	57	LEU
1	A	59	ARG
1	A	62	GLN
1	A	63	ASN
1	A	69	ARG
1	A	74	LEU
1	A	79	VAL
1	A	83	LYS
1	A	90	ASN
1	A	91	VAL
1	A	96	LYS
1	A	98	LEU
1	A	100	GLU
1	A	109	GLU
1	A	117	GLN
1	A	120	GLN
1	A	122	GLU
1	A	132	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	LEU
1	A	150	ARG
1	A	155	SER
1	A	156	ASN
1	A	170	PHE
1	A	172	LEU
1	A	189	ARG
1	A	192	ARG
1	A	203	LYS
1	A	208	ILE
1	A	217	GLU
1	A	236	LYS
1	A	245	SER
1	A	248	PHE
1	A	250	LYS
1	A	256	VAL
1	A	259	TYR
1	A	272	GLU
1	A	287	ASN
1	A	289	LEU
1	A	290	LYS
1	A	298	LEU
1	A	302	LEU
1	A	304	ILE
1	A	308	LYS
1	A	322	ASN
1	A	336	LYS
1	A	337	ILE
1	A	340	LYS
1	A	341	GLN
1	A	342	LEU
1	A	343	ASP
1	A	345	ARG
1	A	355	LEU
1	A	363	LEU
1	A	364	GLU
2	F	555	LYS
2	F	563	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	28	ASN
1	A	37	GLN
1	A	64	GLN
1	A	66	HIS
1	A	82	HIS
1	A	90	ASN
1	A	114	ASN
1	A	120	GLN
1	A	149	HIS
1	A	156	ASN
1	A	318	HIS
1	A	341	GLN
2	F	561	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	344/370 (92%)	-0.16	10 (2%) 49 51	25, 45, 87, 107	0
2	F	10/11 (90%)	-0.03	1 (10%) 8 6	31, 36, 51, 64	0
All	All	354/381 (92%)	-0.16	11 (3%) 47 48	25, 45, 87, 107	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ILE	3.9
1	A	230	HIS	3.9
1	A	227	GLY	3.8
1	A	228	THR	3.1
1	A	253	GLN	2.7
2	F	563	PHE	2.6
1	A	344	GLU	2.3
1	A	234	TRP	2.2
1	A	116	SER	2.1
1	A	342	LEU	2.1
1	A	7	ASP	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.