



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:16 AM UTC

PDB ID : 3VUL / pdb_00003vul
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

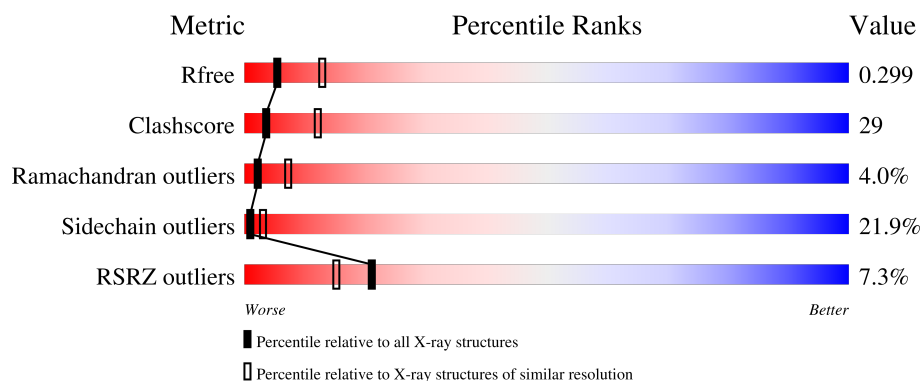
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	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 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 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			

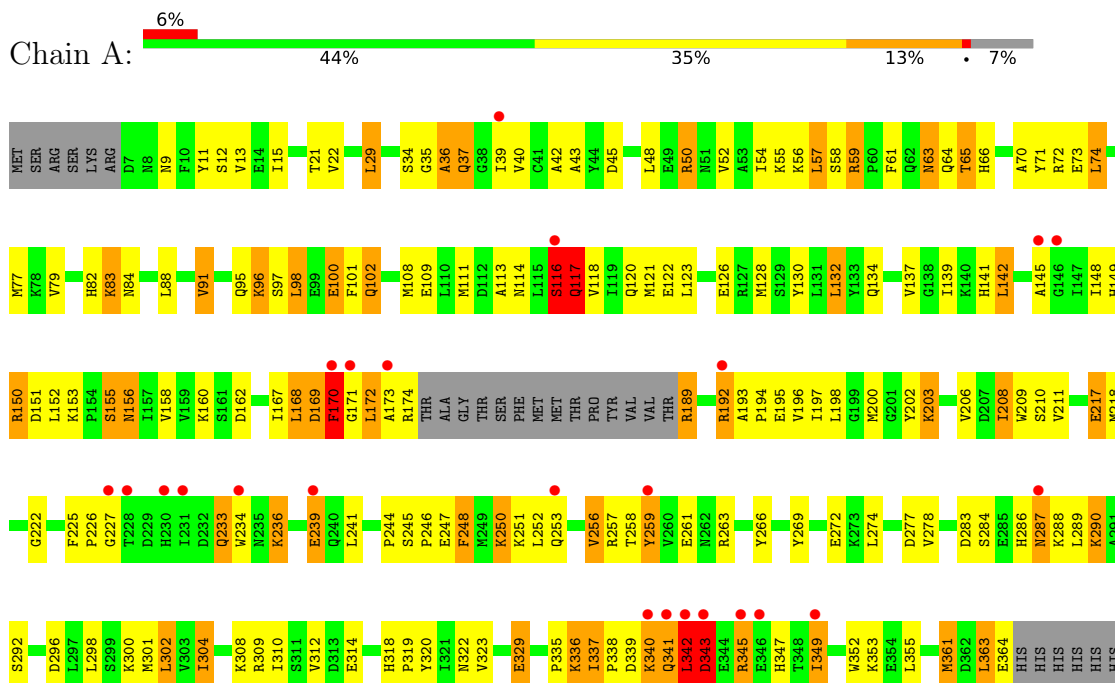
- Molecule 3 is water.

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

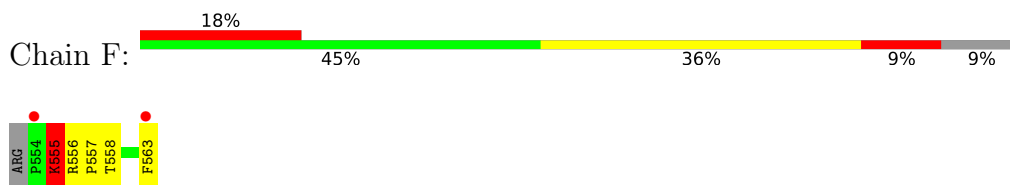
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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



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



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	864 reflections (5.07%)	wwPDB-VP
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 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.96	0/2836	1.18	9/3837 (0.2%)
2	F	1.33	0/86	1.40	1/114 (0.9%)
All	All	0.97	0/2922	1.18	10/3951 (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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	SER	N-CA-C	7.67	121.57	111.75
1	A	116	SER	CA-C-N	7.23	134.71	121.70
1	A	116	SER	C-N-CA	7.23	134.71	121.70
2	F	555	LYS	N-CA-C	5.71	119.54	109.96
1	A	329	GLU	N-CA-C	-5.59	103.99	112.04
1	A	34	SER	N-CA-C	5.27	117.61	107.44
1	A	170	PHE	N-CA-C	-5.17	106.50	114.16
1	A	134	GLN	N-CA-C	5.15	117.56	111.33
1	A	102	GLN	N-CA-C	5.08	120.41	114.62
1	A	248	PHE	N-CA-C	-5.07	107.78	114.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	SER	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	2775	0	2790	168	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	169	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 29.

All (169) 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:82:HIS:HD2	1:A:84:ASN:H	1.07	0.99
1:A:304:ILE:HD12	1:A:304:ILE:H	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:29:LEU:HD22	1:A:43:ALA:HB2	1.56	0.85
1:A:233:GLN:HG3	1:A:234:TRP:H	1.39	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:121:MET:HE3	1:A:123:LEU:HD21	1.64	0.79
1:A:195:GLU:HA	1:A:200:MET:HE3	1.65	0.79
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:211:VAL:HG12	1:A:301:MET:HE3	1.69	0.74
1:A:170:PHE:C	1:A:172:LEU:H	1.97	0.72
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:361:MET:HE3	1:A:361:MET:HA	1.73	0.71
1:A:233:GLN:HG3	1:A:234:TRP:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:HIS:HD2	1:A:151:ASP:H	1.42	0.68
1:A:338:PRO:C	1:A:340:LYS:H	2.02	0.67
1:A:37:GLN:H	1:A:37:GLN:NE2	1.92	0.67
1:A:169:ASP:O	1:A:170:PHE:CD1	2.47	0.67
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
1:A:156:ASN:HD22	1:A:156:ASN:C	2.05	0.65
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: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:111:MET:CE	1:A:160:LYS:HB2	2.29	0.61
1:A:148:ILE:H	1:A:174:ARG:C	2.09	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: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:283:ASP:CG	1:A:290:LYS:HG2	2.29	0.58
1:A:128:MET:O	1:A:132:LEU:HD22	2.04	0.57
1:A:288:LYS:HD2	1:A:323:VAL:HG12	1.85	0.57
1:A:244:PRO:HB2	1:A:248:PHE:CD2	2.40	0.57
1:A:290:LYS:HZ3	1:A:292:SER:HB3	1.68	0.57
1:A:114:ASN:HD22	1:A:155:SER:HA	1.70	0.56
1:A:77:MET:HE1	1:A:108:MET:HG2	1.87	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:259:TYR:C	1:A:259:TYR:CD1	2.83	0.55
1:A:208:ILE:HG23	1:A:301:MET:CG	2.36	0.55
1:A:338:PRO:C	1:A:340:LYS:N	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:114:ASN:ND2	1:A:155:SER:HA	2.21	0.53
1:A:145:ALA:CB	1:A:335:PRO:HG2	2.39	0.53
1:A:111:MET:HE3	1:A:160:LYS:HB2	1.90	0.52
1:A:151:ASP:CG	1:A:151:ASP:O	2.53	0.52
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:170:PHE:C	1:A:172:LEU:N	2.67	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:277:ASP:O	1:A:278:VAL:C	2.54	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:340:LYS:NZ	1:A:341:GLN:HB2	2.26	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:211:VAL:HG12	1:A:301:MET:CE	2.40	0.48
1:A:342:LEU:O	1:A:343:ASP:C	2.57	0.48
1:A:63:ASN:HD22	1:A:66:HIS:CD2	2.31	0.48
1:A:290:LYS:HZ3	1:A:292:SER:CB	2.26	0.48
1:A:310:ILE:HG13	1:A:314:GLU:HB2	1.95	0.48
1:A:202:TYR:O	1:A:203:LYS:HD2	2.13	0.48
1:A:304:ILE:HD12	1:A:304:ILE:N	2.12	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:45:ASP:OD1	1:A:45:ASP:C	2.57	0.47
1:A:63:ASN:ND2	1:A:66:HIS:HD2	2.13	0.47
1:A:70:ALA:O	1:A:74:LEU:HD22	2.15	0.47
1:A:83:LYS:HE3	1:A:329:GLU:HG2	1.96	0.47
1:A:336:LYS:O	1:A:336:LYS:HG3	2.14	0.47
1:A:37:GLN:HE21	1:A:37:GLN:H	1.63	0.47
1:A:111:MET:HE1	1:A:160:LYS:HB2	1.96	0.47
1:A:170:PHE:CB	1:A:173:ALA:HB3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:NE2	1:A:335:PRO:HD3	2.30	0.46
1:A:310:ILE:HD13	1:A:310:ILE:HG21	1.66	0.46
1:A:247:GLU:HG2	1:A:247:GLU:O	2.14	0.46
1:A:59:ARG:NH1	1:A:102:GLN:HB3	2.31	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: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:209:TRP:O	1:A:210:SER:C	2.58	0.46
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:361:MET:HA	1:A:361:MET:CE	2.45	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:11:TYR:O	1:A:21:THR:HA	2.17	0.44
1:A:128:MET:HG3	1:A:218:MET:HE2	1.99	0.44
1:A:296:ASP:OD2	1:A:318:HIS:HE1	2.00	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:111:MET:HG3	1:A:158:VAL:CG2	2.48	0.44
1:A:150:ARG:CZ	1:A:150:ARG:HB2	2.47	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:58:SER:O	1:A:59:ARG:C	2.61	0.44
1:A:246:PRO:C	1:A:248:PHE:H	2.26	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:233:GLN:O	1:A:234:TRP:C	2.62	0.43
1:A:142:LEU:HD12	1:A:142:LEU:HA	1.80	0.43
1:A:352:TRP:O	1:A:353:LYS:C	2.62	0.43
1:A:21:THR:C	1:A:22:VAL:HG13	2.44	0.42
1:A:241:LEU:HD11	1:A:302:LEU:HD22	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ARG:HD3	1:A:52:VAL:HG12	2.00	0.42
1:A:153:LYS:H	1:A:156:ASN:ND2	2.16	0.42
1:A:250:LYS:C	1:A:252:LEU:N	2.77	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:88:LEU:HD11	1:A:91:VAL:HG12	2.02	0.41
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:37:GLN:O	1:A:57:LEU:HD23	2.21	0.41
1:A:345:ARG:HD3	1:A:347:HIS:NE2	2.35	0.41
1:A:284:SER:C	1:A:286:HIS:N	2.78	0.41
1:A:198:LEU:HD12	1:A:200:MET:CE	2.50	0.41
1:A:150:ARG:HH11	1:A:174:ARG:HG2	1.85	0.41
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:283:ASP:OD1	1:A:290:LYS:HG2	2.20	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:341:GLN:CD	1:A:342:LEU:N	2.79	0.41
1:A:341:GLN:CD	1:A:341:GLN:C	2.90	0.40
1:A:151:ASP:OD2	1:A:172:LEU:HG	2.21	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 [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	340/370 (92%)	294 (86%)	32 (9%)	14 (4%)	2	7
2	F	8/11 (73%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	348/381 (91%)	302 (87%)	32 (9%)	14 (4%)	2 7

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
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%)	238 (78%)	67 (22%)	1 3
2	F	10/11 (91%)	8 (80%)	2 (20%)	1 4
All	All	315/342 (92%)	246 (78%)	69 (22%)	1 3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	13	VAL
1	A	15	ILE
1	A	29	LEU

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Mol	Chain	Res	Type
1	A	37	GLN
1	A	39	ILE
1	A	48	LEU
1	A	50	ARG
1	A	54	ILE
1	A	57	LEU
1	A	59	ARG
1	A	63	ASN
1	A	73	GLU
1	A	74	LEU
1	A	79	VAL
1	A	83	LYS
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	126	GLU
1	A	132	LEU
1	A	137	VAL
1	A	142	LEU
1	A	155	SER
1	A	156	ASN
1	A	168	LEU
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	233	GLN
1	A	236	LYS
1	A	239	GLU
1	A	245	SER
1	A	250	LYS
1	A	256	VAL
1	A	258	THR
1	A	259	TYR

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Mol	Chain	Res	Type
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	349	ILE
1	A	355	LEU
1	A	361	MET
1	A	363	LEU
1	A	364	GLU
2	F	555	LYS
2	F	563	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	GLN
1	A	64	GLN
1	A	66	HIS
1	A	81	ASN
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	235	ASN
1	A	240	GLN
1	A	318	HIS
1	A	341	GLN

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Mol	Chain	Res	Type
2	F	561	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 oligosaccharides 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

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%)	0.33	24 (6%) 22 16	25, 45, 87, 107	0
2	F	10/11 (90%)	0.77	2 (20%) 3 2	31, 36, 51, 64	0
All	All	354/381 (92%)	0.35	26 (7%) 21 15	25, 45, 87, 107	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	ILE	5.2
1	A	230	HIS	4.6
1	A	349	ILE	4.4
1	A	228	THR	4.0
1	A	170	PHE	3.8
1	A	39	ILE	3.7
1	A	239	GLU	3.6
1	A	342	LEU	3.4
2	F	554	PRO	3.4
1	A	345	ARG	3.2
2	F	563	PHE	3.2
1	A	346	GLU	3.2
1	A	116	SER	3.1
1	A	259	TYR	3.1
1	A	171	GLY	3.1
1	A	227	GLY	3.0
1	A	234	TRP	2.9
1	A	192	ARG	2.7
1	A	173	ALA	2.7
1	A	253	GLN	2.4
1	A	341	GLN	2.4
1	A	340	LYS	2.2
1	A	287	ASN	2.0
1	A	146	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	145	ALA	2.0
1	A	343	ASP	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 oligosaccharides 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.