



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

PDB ID : 3VUD  
Title : Crystal structure of a cysteine-deficient mutant M1 in MAP kinase JNK1  
Authors : Nakaniwa, T.; Kinoshita, T.; Inoue, T.  
Deposited on : 2012-06-28  
Resolution : 3.50 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](mailto: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.

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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

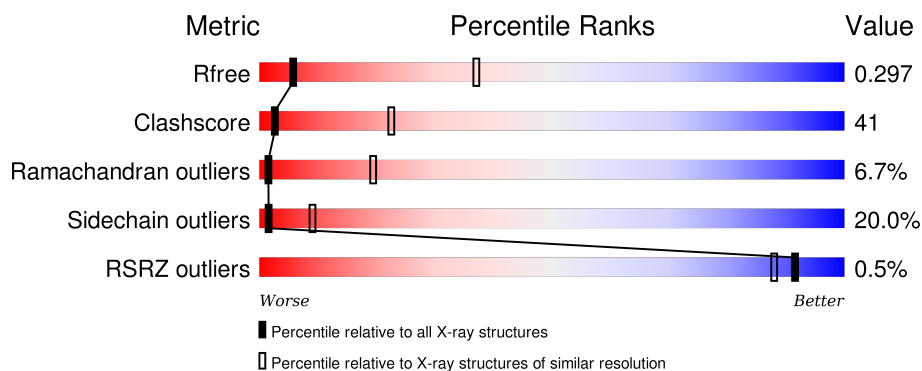
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 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	370	
2	F	11	

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
3	SO4	A	401	-	X	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2947 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	355	Total	C	N	O	S	0	0	0
			2849	1824	480	527	18			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

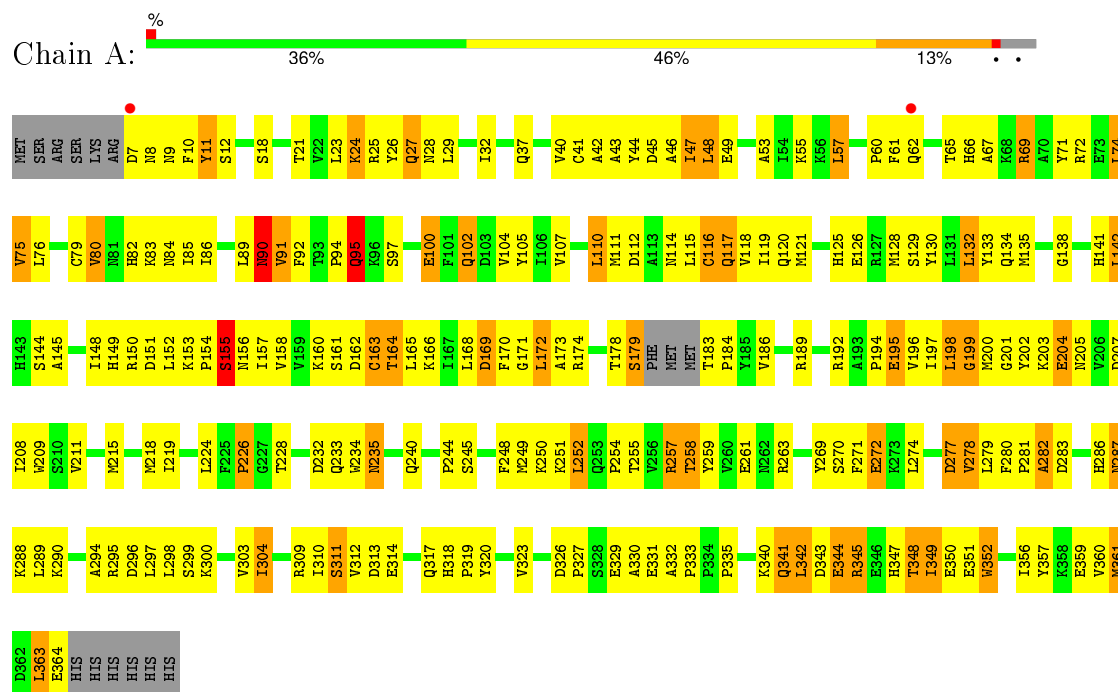
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	O	0	0
			9	9		

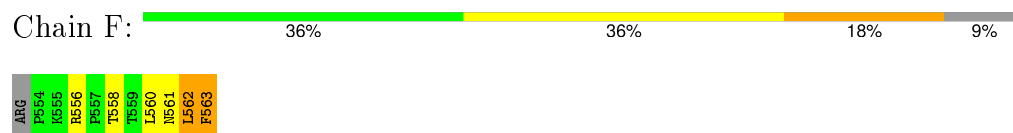
### 3 Residue-property plots

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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.10 Å   170.10 Å   87.98 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	31.73 – 3.50 31.73 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.73-3.50) 99.7 (31.73-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.62 (at 3.47 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.200   ,   0.293 0.203   ,   0.297	Depositor DCC
$R_{free}$ test set	389 reflections (4.87%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 67.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 8385 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	2947	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: 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	0.64	2/2912 (0.1%)	0.82	2/3942 (0.1%)
2	F	0.66	0/86	1.02	0/114
All	All	0.64	2/2998 (0.1%)	0.83	2/4056 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	TRP	CD2-CE2	5.37	1.47	1.41
1	A	352	TRP	CD2-CE2	5.24	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	A	142	LEU	CA-CB-CG	5.76	128.54	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2849	0	2853	237	0
2	F	84	0	91	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	3	0
4	A	9	0	0	4	0
All	All	2947	0	2944	242	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 41.

All (242) 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:71:TYR:HE2	1:A:341:GLN:HG3	1.05	1.12
1:A:71:TYR:CE2	1:A:341:GLN:HG3	1.92	1.03
1:A:125:HIS:CD2	1:A:281:PRO:HG2	1.97	0.99
1:A:304:ILE:HD12	1:A:304:ILE:H	1.34	0.92
1:A:125:HIS:HD2	1:A:281:PRO:HG2	1.32	0.90
1:A:361:MET:HA	1:A:361:MET:CE	1.99	0.90
1:A:318:HIS:HD2	1:A:320:TYR:H	1.21	0.88
1:A:149:HIS:HD2	1:A:151:ASP:H	1.23	0.85
1:A:69:ARG:HH21	1:A:72:ARG:HH12	1.25	0.84
1:A:348:THR:HG22	1:A:351:GLU:H	1.43	0.83
1:A:344:GLU:OE2	1:A:345:ARG:HG3	1.80	0.82
1:A:172:LEU:H	1:A:172:LEU:HD13	1.45	0.80
1:A:348:THR:CG2	1:A:351:GLU:H	1.95	0.80
1:A:128:MET:O	1:A:132:LEU:HD22	1.82	0.79
1:A:114:ASN:HB2	1:A:157:ILE:O	1.83	0.79
1:A:25:ARG:CZ	1:A:47:ILE:HD12	2.13	0.77
1:A:82:HIS:HD2	1:A:84:ASN:H	1.30	0.77
1:A:94:PRO:HD2	1:A:95:GLN:HE22	1.50	0.77
1:A:361:MET:HA	1:A:361:MET:HE2	1.64	0.77
1:A:272:GLU:H	1:A:272:GLU:CD	1.88	0.76
1:A:348:THR:HG23	1:A:350:GLU:H	1.51	0.75
1:A:82:HIS:HD2	1:A:84:ASN:N	1.83	0.75
1:A:149:HIS:CD2	1:A:151:ASP:H	2.05	0.74
1:A:89:LEU:O	1:A:90:ASN:HB2	1.88	0.74
1:A:32:ILE:HD11	1:A:40:VAL:HG12	1.70	0.73
1:A:115:LEU:O	1:A:117:GLN:N	2.22	0.73
1:A:198:LEU:O	1:A:200:MET:HG3	1.87	0.73
1:A:61:PHE:HE2	1:A:102:GLN:HA	1.52	0.72
1:A:172:LEU:HD22	1:A:173:ALA:H	1.54	0.72
1:A:71:TYR:O	1:A:75:VAL:HG23	1.90	0.72
1:A:162:ASP:OD1	1:A:164:THR:OG1	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ASN:ND2	1:A:290:LYS:HE2	2.06	0.70
1:A:198:LEU:HD12	1:A:200:MET:CE	2.22	0.70
1:A:263:ARG:HA	1:A:263:ARG:HH11	1.57	0.69
1:A:46:ALA:O	1:A:49:GLU:HG3	1.93	0.69
1:A:178:THR:HA	1:A:179:SER:C	2.13	0.68
1:A:149:HIS:HD2	1:A:151:ASP:N	1.90	0.68
1:A:172:LEU:N	1:A:172:LEU:HD13	2.08	0.68
1:A:270:SER:HB2	1:A:272:GLU:OE2	1.94	0.67
1:A:215:MET:O	1:A:218:MET:HB2	1.94	0.67
2:F:560:LEU:HD12	2:F:561:ASN:H	1.60	0.65
1:A:318:HIS:CD2	1:A:320:TYR:H	2.09	0.65
1:A:29:LEU:HD22	1:A:43:ALA:HB2	1.77	0.65
1:A:114:ASN:ND2	1:A:155:SER:HA	2.12	0.64
1:A:115:LEU:HB2	1:A:154:PRO:HA	1.79	0.64
1:A:71:TYR:HE2	1:A:341:GLN:CG	1.95	0.64
1:A:310:ILE:HG13	1:A:314:GLU:HB3	1.79	0.64
1:A:348:THR:HG22	1:A:351:GLU:CB	2.28	0.63
1:A:272:GLU:HA	1:A:295:ARG:NE	2.14	0.63
1:A:26:TYR:HA	1:A:44:TYR:O	1.99	0.63
1:A:347:HIS:HB2	1:A:352:TRP:CE2	2.34	0.63
1:A:71:TYR:O	1:A:74:LEU:HB2	1.99	0.62
1:A:287:ASN:HD22	1:A:290:LYS:HE2	1.64	0.62
1:A:60:PRO:O	1:A:66:HIS:HB3	1.98	0.62
1:A:61:PHE:CE2	1:A:102:GLN:HA	2.34	0.62
1:A:153:LYS:O	1:A:157:ILE:HD12	1.98	0.62
1:A:249:MET:O	1:A:251:LYS:N	2.33	0.62
1:A:148:ILE:O	1:A:173:ALA:HA	2.00	0.61
1:A:304:ILE:N	1:A:304:ILE:HD12	2.10	0.61
1:A:76:LEU:O	1:A:80:VAL:HB	2.01	0.61
1:A:97:SER:HA	1:A:357:TYR:OH	2.00	0.60
1:A:82:HIS:CD2	1:A:84:ASN:N	2.69	0.60
1:A:132:LEU:O	1:A:133:TYR:C	2.40	0.60
1:A:277:ASP:O	1:A:280:PHE:N	2.35	0.60
1:A:361:MET:HA	1:A:361:MET:HE3	1.84	0.59
1:A:82:HIS:CD2	1:A:84:ASN:H	2.16	0.59
1:A:94:PRO:HD2	1:A:95:GLN:NE2	2.14	0.59
1:A:352:TRP:O	1:A:356:ILE:HG12	2.03	0.58
1:A:172:LEU:HD22	1:A:173:ALA:N	2.18	0.58
1:A:95:GLN:H	1:A:95:GLN:NE2	2.01	0.58
1:A:287:ASN:O	1:A:289:LEU:N	2.33	0.58
1:A:271:PHE:CZ	1:A:299:SER:HA	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:TYR:CE1	1:A:263:ARG:HD3	2.38	0.57
1:A:341:GLN:HE21	1:A:341:GLN:C	2.06	0.57
1:A:348:THR:HG22	1:A:351:GLU:HB2	1.87	0.57
1:A:342:LEU:O	1:A:345:ARG:HD2	2.04	0.57
1:A:153:LYS:HG2	1:A:156:ASN:HB2	1.86	0.57
1:A:294:ALA:HB2	1:A:320:TYR:CE1	2.39	0.57
1:A:232:ASP:HA	1:A:235:ASN:ND2	2.19	0.57
1:A:149:HIS:HE1	1:A:168:LEU:O	1.86	0.57
1:A:257:ARG:HD3	1:A:261:GLU:OE2	2.04	0.57
1:A:57:LEU:HD12	1:A:57:LEU:H	1.69	0.57
1:A:57:LEU:HD12	1:A:57:LEU:N	2.20	0.57
1:A:263:ARG:N	1:A:263:ARG:HD2	2.20	0.56
1:A:134:GLN:O	1:A:135:MET:C	2.39	0.56
1:A:114:ASN:HD21	1:A:155:SER:HA	1.71	0.56
1:A:171:GLY:N	1:A:172:LEU:HD13	2.19	0.56
1:A:348:THR:H	1:A:351:GLU:HB2	1.71	0.56
1:A:189:ARG:HD3	3:A:401:SO4:O1	2.06	0.56
1:A:90:ASN:HB3	1:A:107:VAL:HB	1.88	0.56
1:A:349:ILE:HG13	1:A:350:GLU:HG2	1.87	0.55
2:F:560:LEU:HD12	2:F:561:ASN:N	2.21	0.55
1:A:90:ASN:HD22	1:A:91:VAL:N	2.04	0.55
1:A:326:ASP:HB3	1:A:329:GLU:OE1	2.05	0.55
1:A:132:LEU:O	1:A:135:MET:HB2	2.07	0.55
1:A:162:ASP:O	1:A:163:CYS:CB	2.53	0.55
1:A:357:TYR:O	1:A:361:MET:HG2	2.07	0.55
1:A:69:ARG:HH21	1:A:72:ARG:NH1	2.02	0.54
1:A:178:THR:HG23	1:A:201:GLY:HA2	1.90	0.54
1:A:71:TYR:HA	1:A:74:LEU:HD23	1.89	0.54
1:A:149:HIS:O	1:A:172:LEU:HD23	2.07	0.54
1:A:286:HIS:O	1:A:287:ASN:O	2.26	0.54
1:A:277:ASP:HA	1:A:280:PHE:HD2	1.73	0.54
1:A:254:PRO:HG2	1:A:255:THR:H	1.73	0.54
1:A:348:THR:HG22	1:A:351:GLU:N	2.18	0.53
1:A:174:ARG:HD3	1:A:202:TYR:OH	2.08	0.53
1:A:341:GLN:HE21	1:A:342:LEU:N	2.06	0.53
1:A:129:SER:HB2	1:A:320:TYR:CE2	2.43	0.53
1:A:271:PHE:HA	1:A:274:LEU:HB2	1.90	0.52
1:A:310:ILE:CG1	1:A:314:GLU:HB3	2.39	0.52
1:A:32:ILE:HG21	1:A:42:ALA:HB2	1.91	0.52
1:A:95:GLN:N	1:A:95:GLN:HE21	2.08	0.51
1:A:69:ARG:NH2	1:A:150:ARG:NH2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ARG:HH22	1:A:48:LEU:HD22	1.75	0.51
1:A:215:MET:HG2	1:A:219:ILE:HD11	1.91	0.51
1:A:204:GLU:N	1:A:204:GLU:OE1	2.37	0.51
1:A:91:VAL:CG2	1:A:363:LEU:HB3	2.40	0.51
1:A:95:GLN:N	1:A:95:GLN:NE2	2.58	0.51
1:A:25:ARG:NH2	1:A:48:LEU:HD22	2.26	0.51
1:A:27:GLN:HB2	1:A:28:ASN:ND2	2.26	0.51
1:A:311:SER:HA	4:A:506:HOH:O	2.11	0.51
1:A:89:LEU:O	1:A:90:ASN:CB	2.59	0.50
1:A:341:GLN:C	1:A:342:LEU:HG	2.32	0.50
1:A:194:PRO:C	1:A:196:VAL:H	2.15	0.50
1:A:154:PRO:C	1:A:156:ASN:H	2.15	0.50
1:A:205:ASN:HD22	1:A:309:ARG:HB3	1.77	0.50
1:A:10:PHE:O	1:A:11:TYR:HB3	2.12	0.50
1:A:85:ILE:O	1:A:166:LYS:HD2	2.11	0.50
1:A:297:LEU:O	1:A:298:LEU:C	2.50	0.50
1:A:69:ARG:NH1	1:A:183:THR:OG1	2.45	0.50
1:A:198:LEU:HD11	1:A:234:TRP:CH2	2.47	0.50
1:A:287:ASN:C	1:A:289:LEU:H	2.15	0.50
1:A:194:PRO:HA	1:A:197:ILE:HD12	1.93	0.49
1:A:207:ASP:O	1:A:211:VAL:HG23	2.11	0.49
1:A:348:THR:HG22	1:A:351:GLU:HG3	1.94	0.49
1:A:249:MET:C	1:A:251:LYS:H	2.16	0.49
1:A:277:ASP:C	1:A:279:LEU:N	2.66	0.49
1:A:204:GLU:H	1:A:204:GLU:CD	2.14	0.49
1:A:154:PRO:O	1:A:156:ASN:N	2.46	0.49
1:A:90:ASN:HB3	1:A:107:VAL:CG2	2.42	0.49
1:A:60:PRO:O	1:A:66:HIS:CB	2.60	0.48
1:A:118:VAL:C	1:A:120:GLN:N	2.66	0.48
1:A:84:ASN:O	1:A:166:LYS:HA	2.13	0.48
1:A:240:GLN:HB3	1:A:274:LEU:HD21	1.95	0.48
1:A:160:LYS:HA	4:A:504:HOH:O	2.13	0.48
1:A:303:VAL:HB	1:A:309:ARG:HG3	1.95	0.48
1:A:245:SER:O	1:A:249:MET:HG2	2.14	0.48
1:A:145:ALA:HB2	1:A:335:PRO:HD2	1.96	0.48
1:A:277:ASP:O	1:A:279:LEU:N	2.46	0.47
1:A:91:VAL:HG21	1:A:363:LEU:CB	2.45	0.47
1:A:57:LEU:HD13	1:A:104:VAL:HB	1.96	0.47
1:A:115:LEU:O	1:A:116:CYS:C	2.53	0.47
1:A:198:LEU:HD12	1:A:200:MET:HE2	1.93	0.47
1:A:195:GLU:HA	1:A:200:MET:SD	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HG3	1:A:158:VAL:CG2	2.45	0.46
1:A:69:ARG:HB3	1:A:171:GLY:O	2.14	0.46
1:A:287:ASN:C	1:A:289:LEU:N	2.68	0.46
1:A:198:LEU:HD13	1:A:252:LEU:HD21	1.97	0.46
1:A:332:ALA:HB1	1:A:333:PRO:CD	2.46	0.46
1:A:10:PHE:CZ	1:A:94:PRO:HA	2.51	0.46
1:A:224:LEU:O	1:A:226:PRO:HD3	2.15	0.46
1:A:263:ARG:HA	1:A:263:ARG:NH1	2.29	0.46
2:F:561:ASN:HD21	2:F:563:PHE:HB3	1.81	0.46
1:A:329:GLU:CD	2:F:556:ARG:HH22	2.18	0.46
1:A:85:ILE:HG23	1:A:170:PHE:HZ	1.81	0.46
1:A:29:LEU:HD23	1:A:29:LEU:N	2.31	0.45
1:A:95:GLN:HB3	1:A:100:GLU:HB3	1.99	0.45
1:A:91:VAL:HG21	1:A:363:LEU:HB3	1.99	0.45
1:A:114:ASN:O	1:A:115:LEU:C	2.55	0.45
1:A:40:VAL:HG22	1:A:55:LYS:HG3	1.98	0.45
1:A:23:LEU:HB3	1:A:25:ARG:HG2	1.98	0.45
1:A:25:ARG:HB2	1:A:47:ILE:HG13	1.99	0.45
1:A:356:ILE:O	1:A:360:VAL:HG23	2.17	0.45
1:A:61:PHE:HA	1:A:67:ALA:HB2	1.99	0.45
1:A:117:GLN:HA	1:A:120:GLN:HB2	1.98	0.44
1:A:232:ASP:HA	1:A:235:ASN:HD21	1.81	0.44
1:A:171:GLY:H	1:A:172:LEU:HD13	1.81	0.44
1:A:296:ASP:O	1:A:299:SER:OG	2.29	0.44
1:A:69:ARG:O	1:A:171:GLY:HA2	2.18	0.44
1:A:348:THR:HG22	1:A:351:GLU:CG	2.48	0.44
1:A:320:TYR:CD2	1:A:320:TYR:O	2.71	0.44
1:A:71:TYR:HE1	1:A:359:GLU:HB2	1.83	0.44
1:A:198:LEU:HD21	1:A:234:TRP:CE3	2.52	0.44
1:A:120:GLN:OE1	1:A:120:GLN:HA	2.18	0.43
1:A:297:LEU:O	1:A:300:LYS:N	2.41	0.43
1:A:138:GLY:O	1:A:141:HIS:HB3	2.19	0.43
1:A:172:LEU:CD2	1:A:173:ALA:N	2.81	0.43
1:A:269:TYR:HB2	1:A:274:LEU:HG	2.01	0.43
1:A:53:ALA:HB2	1:A:110:LEU:HD12	2.01	0.43
1:A:169:ASP:O	1:A:172:LEU:HD21	2.19	0.43
1:A:82:HIS:CD2	1:A:84:ASN:HB2	2.54	0.43
1:A:249:MET:C	1:A:251:LYS:N	2.73	0.43
1:A:271:PHE:CE1	1:A:299:SER:HA	2.54	0.43
1:A:92:PHE:CE1	1:A:105:TYR:CD1	3.07	0.43
1:A:130:TYR:O	1:A:133:TYR:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ILE:HD13	1:A:298:LEU:HD11	2.00	0.42
1:A:189:ARG:HA	1:A:192:ARG:NE	2.34	0.42
1:A:272:GLU:HA	1:A:295:ARG:HE	1.82	0.42
1:A:233:GLN:O	1:A:234:TRP:C	2.56	0.42
1:A:327:PRO:HA	1:A:330:ALA:HB3	2.01	0.42
1:A:189:ARG:NH1	3:A:401:SO4:O4	2.52	0.42
1:A:118:VAL:C	1:A:120:GLN:H	2.23	0.42
1:A:118:VAL:O	1:A:120:GLN:N	2.52	0.42
1:A:304:ILE:H	1:A:304:ILE:CD1	2.00	0.42
1:A:257:ARG:O	1:A:258:THR:C	2.58	0.42
1:A:66:HIS:CE1	4:A:501:HOH:O	2.73	0.42
1:A:112:ASP:N	4:A:504:HOH:O	2.34	0.42
1:A:29:LEU:HA	1:A:42:ALA:O	2.19	0.42
1:A:45:ASP:O	1:A:49:GLU:HA	2.20	0.42
1:A:62:GLN:HE21	1:A:66:HIS:CE1	2.38	0.42
1:A:272:GLU:HA	1:A:295:ARG:CD	2.50	0.42
1:A:117:GLN:HE21	1:A:117:GLN:HB2	1.43	0.41
1:A:277:ASP:C	1:A:279:LEU:H	2.22	0.41
1:A:226:PRO:O	1:A:233:GLN:NE2	2.53	0.41
1:A:300:LYS:O	1:A:310:ILE:HG22	2.20	0.41
1:A:172:LEU:CD1	1:A:172:LEU:N	2.74	0.41
1:A:23:LEU:O	1:A:24:LYS:C	2.59	0.41
2:F:561:ASN:C	2:F:562:LEU:HG	2.38	0.41
1:A:154:PRO:C	1:A:156:ASN:N	2.74	0.41
1:A:82:HIS:HB2	1:A:141:HIS:ND1	2.35	0.41
1:A:192:ARG:NH2	3:A:401:SO4:O1	2.54	0.41
1:A:203:LYS:HB3	1:A:204:GLU:OE1	2.21	0.41
1:A:244:PRO:HB2	1:A:248:PHE:CD2	2.56	0.41
1:A:86:ILE:HD12	1:A:86:ILE:HA	1.84	0.41
1:A:281:PRO:C	1:A:282:ALA:O	2.59	0.41
1:A:348:THR:HG23	1:A:351:GLU:H	1.79	0.41
1:A:198:LEU:O	1:A:199:GLY:C	2.58	0.41
1:A:263:ARG:HA	1:A:263:ARG:HD2	1.80	0.41
1:A:26:TYR:HE1	1:A:45:ASP:OD2	2.04	0.41
1:A:326:ASP:O	1:A:329:GLU:N	2.45	0.41
1:A:97:SER:O	1:A:100:GLU:N	2.53	0.41
1:A:115:LEU:O	1:A:118:VAL:N	2.31	0.40
1:A:32:ILE:CG2	1:A:42:ALA:HB2	2.51	0.40
2:F:561:ASN:ND2	2:F:563:PHE:HB3	2.37	0.40
1:A:82:HIS:O	1:A:84:ASN:N	2.54	0.40
1:A:205:ASN:O	1:A:309:ARG:NH1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:HIS:HA	1:A:319:PRO:HD2	1.56	0.40
1:A:44:TYR:CE2	1:A:46:ALA:HA	2.57	0.40
1:A:326:ASP:C	1:A:326:ASP:OD1	2.59	0.40
1:A:149:HIS:O	1:A:150:ARG:HB2	2.21	0.40
1:A:44:TYR:OH	1:A:49:GLU:HG2	2.21	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.69	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	351/370 (95%)	263 (75%)	64 (18%)	24 (7%)	1	19
2	F	8/11 (73%)	8 (100%)	0	0	100	100
All	All	359/381 (94%)	271 (76%)	64 (18%)	24 (7%)	1	19

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	116	CYS
1	A	169	ASP
1	A	184	PRO
1	A	199	GLY
1	A	250	LYS
1	A	287	ASN
1	A	349	ILE
1	A	90	ASN
1	A	155	SER
1	A	226	PRO
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	278	VAL
1	A	282	ALA
1	A	288	LYS
1	A	65	THR
1	A	74	LEU
1	A	195	GLU
1	A	119	ILE
1	A	144	SER
1	A	343	ASP
1	A	47	ILE
1	A	95	GLN
1	A	102	GLN

### 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	315/332 (95%)	253 (80%)	62 (20%)	1	9
2	F	10/11 (91%)	7 (70%)	3 (30%)	0	3
All	All	325/343 (95%)	260 (80%)	65 (20%)	1	9

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	8	ASN
1	A	9	ASN
1	A	11	TYR
1	A	12	SER
1	A	18	SER
1	A	21	THR
1	A	24	LYS
1	A	27	GLN
1	A	37	GLN
1	A	41	CYS

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Mol	Chain	Res	Type
1	A	48	LEU
1	A	57	LEU
1	A	75	VAL
1	A	79	CYS
1	A	80	VAL
1	A	90	ASN
1	A	91	VAL
1	A	95	GLN
1	A	100	GLU
1	A	110	LEU
1	A	117	GLN
1	A	121	MET
1	A	126	GLU
1	A	132	LEU
1	A	142	LEU
1	A	152	LEU
1	A	155	SER
1	A	161	SER
1	A	163	CYS
1	A	164	THR
1	A	165	LEU
1	A	172	LEU
1	A	179	SER
1	A	186	VAL
1	A	198	LEU
1	A	204	GLU
1	A	208	ILE
1	A	228	THR
1	A	235	ASN
1	A	257	ARG
1	A	258	THR
1	A	272	GLU
1	A	277	ASP
1	A	278	VAL
1	A	283	ASP
1	A	304	ILE
1	A	311	SER
1	A	312	VAL
1	A	313	ASP
1	A	317	GLN
1	A	323	VAL
1	A	331	GLU

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Mol	Chain	Res	Type
1	A	340	LYS
1	A	341	GLN
1	A	342	LEU
1	A	344	GLU
1	A	345	ARG
1	A	348	THR
1	A	361	MET
1	A	363	LEU
1	A	364	GLU
2	F	558	THR
2	F	562	LEU
2	F	563	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	28	ASN
1	A	62	GLN
1	A	82	HIS
1	A	84	ASN
1	A	90	ASN
1	A	114	ASN
1	A	117	GLN
1	A	125	HIS
1	A	149	HIS
1	A	233	GLN
1	A	240	GLN
1	A	287	ASN
1	A	317	GLN
1	A	318	HIS
1	A	341	GLN
2	F	561	ASN

### 5.3.3 RNA ⓘ

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	$\# Z  > 2$
3	SO4	A	401	-	4,4,4	0.62	0	6,6,6	2.99	4 (66%)

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
3	SO4	A	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SO4	O4-S-O3	-5.31	87.40	108.98
3	A	401	SO4	O4-S-O1	-2.47	87.19	110.19
3	A	401	SO4	O4-S-O2	-2.43	87.59	110.19
3	A	401	SO4	O2-S-O1	3.37	120.16	109.50

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
3	A	401	SO4	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	355/370 (95%)	-0.49	2 (0%) 90 85	29, 55, 100, 124	0
2	F	10/11 (90%)	-0.20	0 100 100	44, 49, 59, 87	0
All	All	365/381 (95%)	-0.48	2 (0%) 91 88	29, 55, 99, 124	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	GLN	2.4
1	A	7	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	A	401	5/5	0.97	0.15	-2.39	64,67,70,71	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.