Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2025 – 10:09 AM EDT

PDB ID	:	9DL0 / pdb_00009dl0
Title	:	Crystal structure of a synthetic Fab (R3H8) in complex with the FRB domain of mTOR
Authors	:	O'Leary, K.M.; Slezak, T.; Kossiakoff, A.A.
Deposited on	:	2024-09-10
Resolution	:	2.00 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:

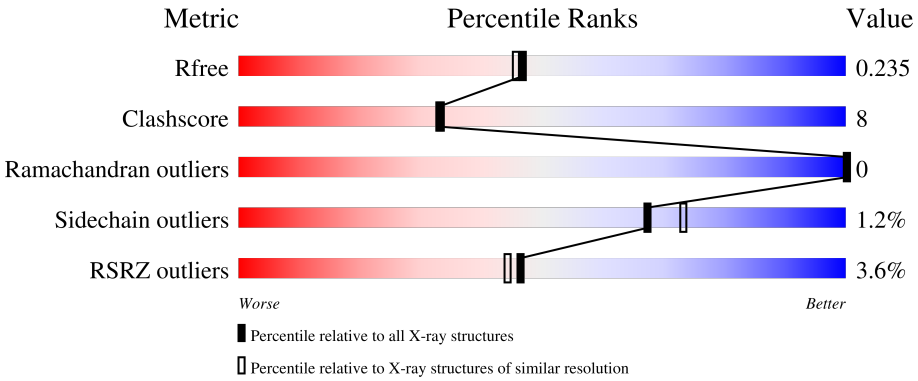
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (2.00-2.00)

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 <=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	224	4% 84% 12%
1	H	224	4% 85% 14%
2	G	98	5% 79% 15% 6%
2	I	98	5% 93% 6%
3	Y	212	87% 13%

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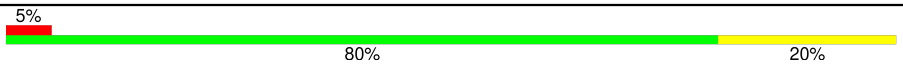
Mol	Chain	Length	Quality of chain
3	Z	212	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8837 atoms, of which 351 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1618	1024	268	320	6			
1	H	224	Total	C	N	O	S	0	0	0
			1656	1045	275	330	6			

- Molecule 2 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	92	Total	C	H	N	O	S	173	0	0
			952	497	173	136	139	7			
2	I	98	Total	C	H	N	O	S	178	0	0
			992	517	178	144	146	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	2020	SER	-	expression tag	UNP P42345
G	2114	GLY	-	expression tag	UNP P42345
G	2115	GLY	-	expression tag	UNP P42345
G	2116	GLY	-	expression tag	UNP P42345
G	2117	GLY	-	expression tag	UNP P42345
I	2020	SER	-	expression tag	UNP P42345
I	2114	GLY	-	expression tag	UNP P42345
I	2115	GLY	-	expression tag	UNP P42345
I	2116	GLY	-	expression tag	UNP P42345
I	2117	GLY	-	expression tag	UNP P42345

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	212	Total	C	N	O	S	0	0	0
			1623	1017	273	328	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	212	Total	C	N	O	S	0	0	0
			1623	1017	273	328	5			

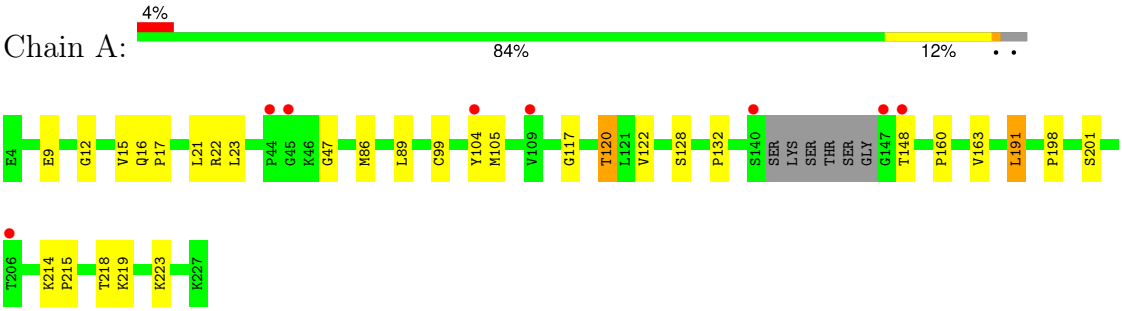
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	G	29	Total	O	0	0
			29	29		
4	H	56	Total	O	0	0
			56	56		
4	I	44	Total	O	0	0
			44	44		
4	Y	102	Total	O	0	0
			102	102		
4	Z	92	Total	O	0	0
			92	92		

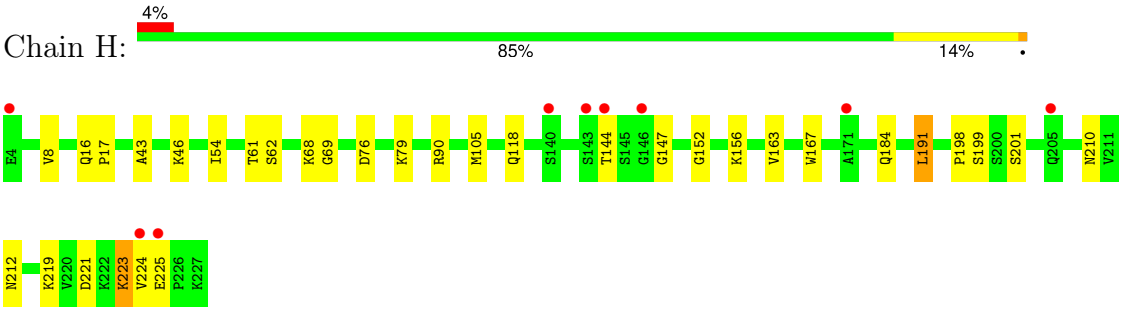
3 Residue-property plots (i)

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.

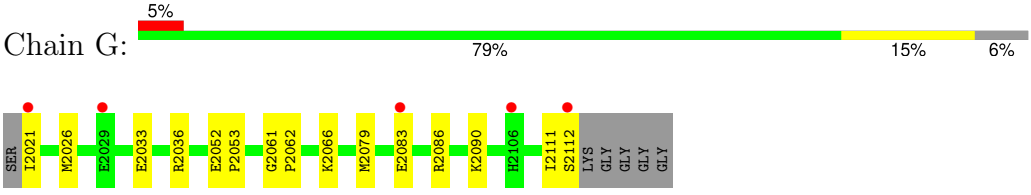
• Molecule 1: Fab heavy chain



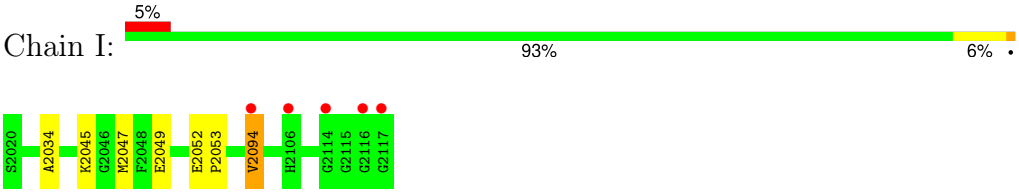
• Molecule 1: Fab heavy chain



• Molecule 2: Serine/threonine-protein kinase mTOR

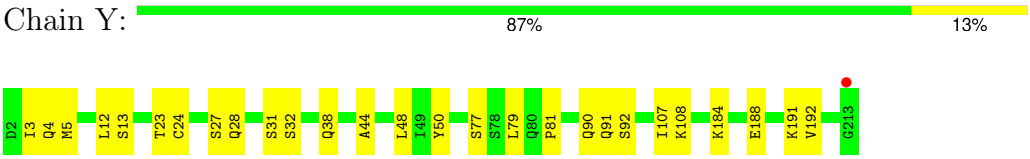


• Molecule 2: Serine/threonine-protein kinase mTOR



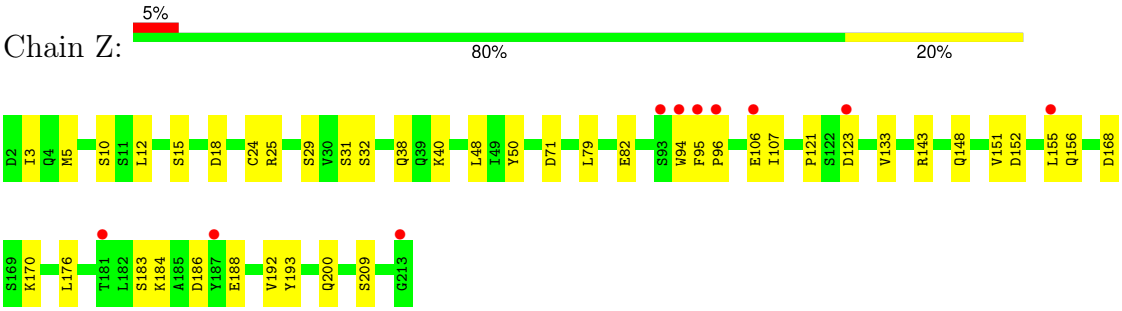
• Molecule 3: Fab light chain

Chain Y:



• Molecule 3: Fab light chain

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	87.61Å 110.04Å 131.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.31 – 2.00 56.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (56.31-2.00) 95.6 (56.31-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.21.1)	Depositor
R, R_{free}	0.205 , 0.234 0.206 , 0.235	Depositor DCC
R_{free} test set	4447 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	37.6	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8837	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/1658	0.55	0/2259
1	H	0.32	0/1697	0.52	0/2312
2	G	0.39	0/801	0.57	0/1078
2	I	0.37	0/836	0.55	0/1121
3	Y	0.41	0/1659	0.64	0/2253
3	Z	0.42	0/1659	0.62	0/2253
All	All	0.37	0/8310	0.58	0/11276

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1618	0	1571	25	0
1	H	1656	0	1610	28	0
2	G	779	173	735	10	0
2	I	814	178	776	9	0
3	Y	1623	0	1582	19	0
3	Z	1623	0	1582	42	0
4	A	50	0	0	1	0
4	G	29	0	0	2	0
4	H	56	0	0	2	0
4	I	44	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Y	102	0	0	1	0
4	Z	92	0	0	0	0
All	All	8486	351	7856	123	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 8.

All (123) 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:H:223:LYS:HD3	1:H:223:LYS:H	1.34	0.91
1:A:16:GLN:HG3	1:A:17:PRO:HD2	1.51	0.90
3:Z:3:ILE:HD11	3:Z:94:TRP:CE2	2.08	0.89
1:A:223:LYS:H	1:A:223:LYS:HD2	1.40	0.86
3:Y:184:LYS:O	3:Y:188:GLU:HG3	1.77	0.84
2:I:2094:VAL:CG1	3:Z:94:TRP:CZ2	2.61	0.83
2:I:2094:VAL:HG11	3:Z:94:TRP:CZ2	2.19	0.77
3:Z:184:LYS:O	3:Z:188:GLU:HG3	1.85	0.77
3:Z:5:MET:HE3	3:Z:24:CYS:SG	2.24	0.76
1:A:132:PRO:HD2	1:A:218:THR:HG21	1.68	0.75
3:Z:3:ILE:HD11	3:Z:94:TRP:CZ2	2.22	0.74
1:H:16:GLN:HG2	1:H:17:PRO:HD2	1.68	0.73
3:Z:79:LEU:HD21	3:Z:107:ILE:HD12	1.70	0.73
3:Z:152:ASP:OD2	3:Z:192:VAL:HG12	1.89	0.72
1:H:223:LYS:HD3	1:H:223:LYS:N	2.06	0.69
1:H:223:LYS:H	1:H:223:LYS:CD	2.05	0.68
3:Z:152:ASP:HA	3:Z:192:VAL:CG1	2.24	0.67
1:A:191:LEU:C	1:A:191:LEU:HD12	2.22	0.65
3:Y:90:GLN:HE22	3:Y:92:SER:HB3	1.62	0.63
3:Z:29:SER:O	3:Z:94:TRP:CH2	2.51	0.63
3:Z:3:ILE:HG12	3:Z:94:TRP:CD1	2.34	0.63
2:I:2094:VAL:HG13	3:Z:94:TRP:CZ2	2.34	0.62
1:H:76:ASP:OD1	1:H:79:LYS:HE3	1.99	0.62
1:A:21:LEU:HD22	1:A:86:MET:HE2	1.82	0.61
3:Z:148:GLN:OE1	3:Z:155:LEU:HD21	1.99	0.61
1:A:198:PRO:HG2	1:A:201:SER:OG	2.00	0.61
1:H:43:ALA:HB3	1:H:46:LYS:HE2	1.82	0.61
1:H:105:MET:HB3	3:Z:50:TYR:CE2	2.36	0.61
3:Z:95:PHE:HB3	3:Z:96:PRO:HD3	1.82	0.61
1:A:21:LEU:HD22	1:A:86:MET:CE	2.31	0.60
3:Y:13:SER:OG	3:Y:108:LYS:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLN:HG3	1:A:17:PRO:CD	2.29	0.59
2:G:2033:GLU:OE1	2:G:2036:ARG:NH1	2.35	0.59
3:Y:31:SER:O	3:Y:31:SER:OG	2.18	0.59
1:H:147:GLY:O	1:H:199:SER:N	2.30	0.59
2:G:2086:ARG:O	2:G:2090:LYS:HE3	2.03	0.58
1:H:8:VAL:HA	1:H:118:GLN:HE22	1.67	0.58
3:Z:29:SER:O	3:Z:94:TRP:HH2	1.86	0.58
3:Y:90:GLN:NE2	3:Y:92:SER:HB3	2.19	0.57
3:Z:168:ASP:OD2	3:Z:170:LYS:HE3	2.04	0.57
3:Y:38:GLN:HB2	3:Y:48:LEU:HD11	1.87	0.57
3:Z:121:PRO:HD3	3:Z:133:VAL:HG22	1.87	0.56
3:Y:191:LYS:HE3	3:Y:192:VAL:HG23	1.89	0.54
1:A:105:MET:HE2	3:Y:50:TYR:CD2	2.44	0.53
3:Y:90:GLN:HE21	3:Y:91:GLN:C	2.17	0.53
2:I:2094:VAL:HG11	3:Z:94:TRP:HZ2	1.71	0.53
1:A:191:LEU:HA	4:A:328:HOH:O	2.08	0.53
3:Z:38:GLN:HB2	3:Z:48:LEU:HD11	1.91	0.53
3:Y:5:MET:HE3	3:Y:24:CYS:SG	2.49	0.53
3:Z:25:ARG:HD2	3:Z:71:ASP:OD1	2.09	0.53
3:Y:31:SER:O	3:Y:32:SER:HB2	2.08	0.52
2:I:2052:GLU:HB3	2:I:2053:PRO:HD3	1.91	0.52
3:Z:31:SER:O	3:Z:32:SER:HB2	2.09	0.52
2:G:2021:ILE:HG23	2:G:2026:MET:SD	2.49	0.52
1:H:62:SER:HB3	3:Z:95:PHE:CE1	2.45	0.52
1:H:191:LEU:C	1:H:191:LEU:HD12	2.34	0.52
1:H:90:ARG:HD2	4:H:349:HOH:O	2.11	0.51
1:H:212:ASN:HD21	1:H:219:LYS:HE2	1.75	0.51
3:Z:106:GLU:CD	3:Z:143:ARG:HH22	2.19	0.51
3:Z:3:ILE:CD1	3:Z:94:TRP:CE2	2.91	0.51
1:A:117:GLY:O	3:Y:44:ALA:HB2	2.11	0.50
3:Z:183:SER:OG	3:Z:186:ASP:OD2	2.28	0.50
1:A:223:LYS:H	1:A:223:LYS:CD	2.16	0.50
3:Y:81:PRO:HA	3:Y:107:ILE:HG13	1.94	0.50
3:Z:152:ASP:HA	3:Z:192:VAL:HG13	1.93	0.50
2:G:2079:MET:O	2:G:2083:GLU:HG3	2.11	0.50
3:Y:12:LEU:C	3:Y:12:LEU:HD12	2.36	0.50
3:Z:123:ASP:N	3:Z:123:ASP:OD1	2.45	0.50
2:G:2079:MET:HE1	4:G:2228:HOH:O	2.12	0.49
1:A:219:LYS:NZ	1:A:219:LYS:HB3	2.27	0.48
1:H:43:ALA:CB	1:H:46:LYS:HE2	2.43	0.48
3:Z:94:TRP:N	3:Z:94:TRP:HE3	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:54:ILE:HD12	1:H:61:THR:HG22	1.94	0.48
1:H:16:GLN:HG2	1:H:17:PRO:CD	2.42	0.48
1:H:144:THR:HG22	1:H:144:THR:O	2.14	0.48
3:Z:3:ILE:HG13	3:Z:94:TRP:CD2	2.48	0.47
1:H:210:ASN:ND2	1:H:221:ASP:OD1	2.37	0.47
1:H:156:LYS:NZ	1:H:184:GLN:HE22	2.13	0.47
1:H:152:GLY:HA2	1:H:167:TRP:CH2	2.50	0.47
3:Z:40:LYS:HE2	3:Z:82:GLU:O	2.15	0.47
1:H:210:ASN:HD22	1:H:221:ASP:CG	2.23	0.46
1:H:224:VAL:C	1:H:225:GLU:HG3	2.40	0.46
1:H:147:GLY:O	1:H:198:PRO:HA	2.16	0.46
1:A:15:VAL:HG11	1:A:89:LEU:HD13	1.97	0.46
3:Z:95:PHE:CD1	3:Z:95:PHE:C	2.90	0.46
1:A:47:GLY:HA3	4:Y:312:HOH:O	2.14	0.46
3:Y:79:LEU:HD21	3:Y:107:ILE:HD12	1.98	0.46
3:Z:79:LEU:HD21	3:Z:107:ILE:CD1	2.43	0.46
3:Y:4:GLN:HB2	3:Y:27:SER:OG	2.17	0.45
1:A:9:GLU:HG3	1:A:99:CYS:SG	2.57	0.45
1:A:12:GLY:H	1:A:120:THR:HG21	1.81	0.45
2:I:2045:LYS:HE2	2:I:2049:GLU:OE2	2.16	0.45
1:H:198:PRO:HG2	1:H:201:SER:OG	2.18	0.44
2:I:2094:VAL:HG11	3:Z:94:TRP:CE2	2.51	0.44
2:I:2034:ALA:HB1	2:I:2047:MET:HG3	1.98	0.44
1:A:86:MET:HE1	1:A:122:VAL:HG21	2.00	0.44
3:Z:155:LEU:HD23	3:Z:156:GLN:O	2.17	0.44
1:H:118:GLN:H	1:H:118:GLN:CD	2.25	0.44
1:A:160:PRO:HD2	1:A:215:PRO:HB2	1.99	0.44
1:H:68:LYS:HD2	1:H:69:GLY:N	2.33	0.43
2:G:2021:ILE:HG23	2:G:2026:MET:CG	2.48	0.43
2:G:2066:LYS:NZ	4:G:2203:HOH:O	2.43	0.43
3:Y:3:ILE:HD12	3:Y:28:GLN:HG2	1.99	0.43
3:Z:176:LEU:C	3:Z:176:LEU:HD23	2.44	0.43
3:Y:23:THR:HG22	3:Y:24:CYS:N	2.34	0.43
2:G:2111:ILE:O	2:G:2112:SER:CB	2.67	0.43
3:Z:12:LEU:C	3:Z:12:LEU:HD12	2.44	0.43
3:Z:79:LEU:CD2	3:Z:107:ILE:HD12	2.45	0.42
1:A:148:THR:O	1:A:148:THR:HG23	2.20	0.42
1:A:21:LEU:HD23	1:A:22:ARG:N	2.35	0.42
1:A:160:PRO:HD2	1:A:215:PRO:CB	2.48	0.42
1:H:90:ARG:CD	4:H:349:HOH:O	2.66	0.42
3:Z:151:VAL:HG22	3:Z:193:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HG	1:A:86:MET:HE2	2.01	0.42
1:A:104:TYR:C	1:A:104:TYR:CD1	2.98	0.42
1:H:212:ASN:ND2	1:H:219:LYS:HE2	2.35	0.42
3:Z:15:SER:O	3:Z:18:ASP:HB2	2.20	0.41
2:I:2094:VAL:CG1	3:Z:94:TRP:HZ2	2.22	0.41
3:Y:191:LYS:HE3	3:Y:192:VAL:CG2	2.50	0.41
1:A:214:LYS:N	1:A:215:PRO:CD	2.84	0.41
3:Z:193:TYR:O	3:Z:209:SER:HA	2.21	0.41
2:G:2052:GLU:HB3	2:G:2053:PRO:HD3	2.03	0.41
2:G:2061:GLY:HA2	2:G:2062:PRO:HD3	1.96	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	214/224 (96%)	210 (98%)	4 (2%)	0	100	100
1	H	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
2	G	90/98 (92%)	90 (100%)	0	0	100	100
2	I	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
3	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
3	Z	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
All	All	1042/1068 (98%)	1015 (97%)	27 (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	181/186 (97%)	177 (98%)	4 (2%)	47 51
1	H	186/186 (100%)	183 (98%)	3 (2%)	58 64
2	G	80/83 (96%)	80 (100%)	0	100 100
2	I	83/83 (100%)	82 (99%)	1 (1%)	67 73
3	Y	187/187 (100%)	186 (100%)	1 (0%)	86 90
3	Z	187/187 (100%)	185 (99%)	2 (1%)	70 76
All	All	904/912 (99%)	893 (99%)	11 (1%)	67 73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	THR
1	A	128	SER
1	A	163	VAL
1	A	191	LEU
1	H	163	VAL
1	H	191	LEU
1	H	223	LYS
2	I	2094	VAL
3	Y	77	SER
3	Z	10	SER
3	Z	200	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	85	GLN
1	A	118	GLN
1	A	177	HIS
1	A	212	ASN
2	G	2071	ASN

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Mol	Chain	Res	Type
1	H	118	GLN
1	H	184	GLN
1	H	212	ASN
2	I	2024	HIS
2	I	2071	ASN
2	I	2082	GLN
2	I	2106	HIS
3	Y	39	GLN
3	Y	90	GLN

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 oligosaccharides 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, 95^{th} 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	218/224 (97%)	0.44	8 (3%)	45	43	30, 46, 69, 92	0
1	H	224/224 (100%)	0.46	9 (4%)	43	41	28, 47, 83, 133	0
2	G	92/98 (93%)	0.30	5 (5%)	32	30	25, 36, 54, 76	0
2	I	98/98 (100%)	0.34	5 (5%)	34	32	24, 35, 61, 69	0
3	Y	212/212 (100%)	0.04	1 (0%)	87	86	27, 38, 58, 76	0
3	Z	212/212 (100%)	0.37	10 (4%)	37	35	23, 40, 83, 92	0
All	All	1056/1068 (98%)	0.33	38 (3%)	46	44	23, 42, 75, 133	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Z	94	TRP	9.3
3	Z	95	PHE	5.2
1	A	44	PRO	4.2
2	G	2021	ILE	3.5
2	G	2112	SER	3.3
2	I	2094	VAL	3.1
1	H	144	THR	3.0
3	Y	213	GLY	2.9
1	H	146	GLY	2.9
3	Z	93	SER	2.8
3	Z	155	LEU	2.8
2	I	2114	GLY	2.8
3	Z	96	PRO	2.7
2	I	2117	GLY	2.7
1	A	206	THR	2.7
1	H	143	SER	2.6
1	A	147	GLY	2.6
2	G	2029	GLU	2.6
1	H	225	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
3	Z	213	GLY	2.5
2	I	2106	HIS	2.5
1	H	171	ALA	2.5
1	A	140	SER	2.4
1	H	224	VAL	2.4
1	A	45	GLY	2.4
3	Z	123	ASP	2.4
1	H	140	SER	2.3
1	A	148	THR	2.2
2	I	2116	GLY	2.2
1	H	205	GLN	2.2
1	H	4	GLU	2.1
1	A	104	TYR	2.1
2	G	2106	HIS	2.1
1	A	109	VAL	2.1
3	Z	106	GLU	2.1
2	G	2083	GLU	2.1
3	Z	181	THR	2.0
3	Z	187	TYR	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 monosaccharides 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.