Full wwPDB X-ray Structure Validation Report (i)

Feb 12, 2017 – 05:55 AM EST

PDB ID : 5L2Q
Title : Serine/threonine-protein kinase 40 (STK40) kinase homology domain
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Deposited on : 2016-08-02
Resolution : 2.53 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
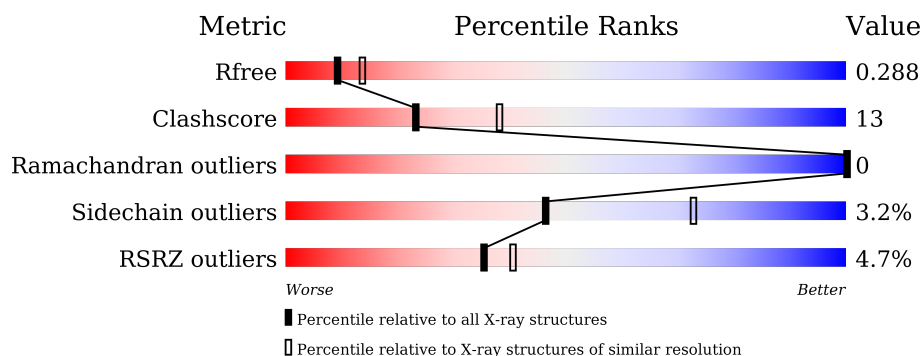with specific help available everywhere you see the (i) symbol.

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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 2.53 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	Percentile Ranks	Value
Rfree		0.288
Clashscore		13
Ramachandran outliers		0
Sidechain outliers		3.2%
RSRZ outliers		4.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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 <=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	320	.% 65% 25% • 8%
1	B	320	2% 66% 22% • 12%
1	C	320	8% 67% 21% • 12%
1	D	320	7% 67% 24% • 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8350 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 Serine/threonine-protein kinase 40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	282	Total	C	N	O	S	5	1	0
			2023	1298	352	362	11			
1	B	282	Total	C	N	O	S	0	0	0
			2072	1320	361	381	10			
1	A	293	Total	C	N	O	S	0	0	0
			2166	1394	376	386	10			
1	D	294	Total	C	N	O	S	0	0	0
			2023	1273	358	381	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	expression tag	UNP Q8N2I9
A	21	SER	-	expression tag	UNP Q8N2I9
B	20	GLY	-	expression tag	UNP Q8N2I9
B	21	SER	-	expression tag	UNP Q8N2I9
C	20	GLY	-	expression tag	UNP Q8N2I9
C	21	SER	-	expression tag	UNP Q8N2I9
D	20	GLY	-	expression tag	UNP Q8N2I9
D	21	SER	-	expression tag	UNP Q8N2I9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	16	Total	O	0	0
			16	16		
2	B	17	Total	O	0	0
			17	17		
2	A	20	Total	O	0	0
			20	20		
2	D	13	Total	O	0	0
			13	13		

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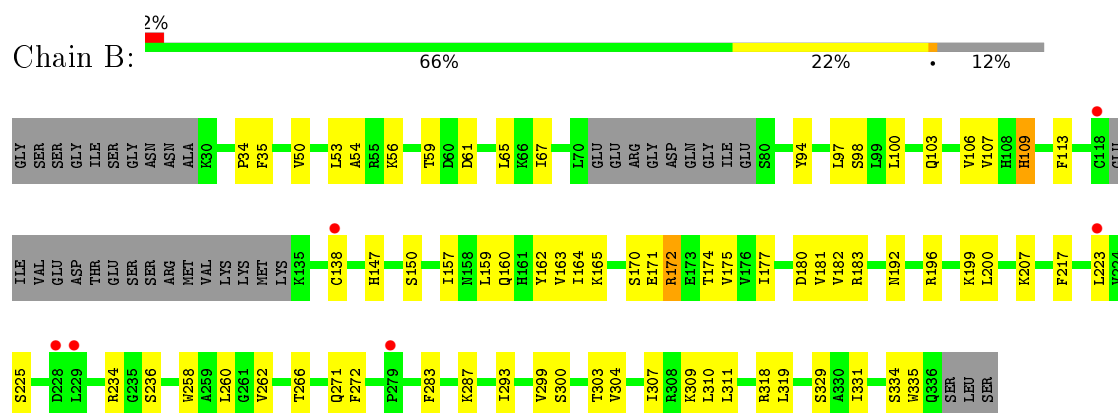 = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Serine/threonine-protein kinase 40

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V224 S225 L229 L230 R234 P249 L260 G261 V262 Y269 P273 F274 Y275 D276 L282 K285 E290 Y291 D296 GLY ARG V299 S300 E301 V304 C305 L306 V312 R318 L319 A320 A321 V324 L328 I331 Q336 SER LEU SER

• Molecule 1: Serine/threonine-protein kinase 40

Chain D:

GLY SER SER GLY ILE SER GLY ASN ASN ALA K30 R31 A32 G33 P34 F35 I36 L37 V50 Q51 C52 L53 A54 R55 T59 D60 D61 F62 Y63 Q64 L65 K66 I67 L68 T69 L70 GLU GLU ARG GLY ASP GLN GLY ILE GLU SER Q81 K87 M88 L89 E93 L96 L99 L100

D104 G105 V106 V107 D115 C118 E119 I120 V121 S126 M129 V130 K131 K132 M133 R136 I137 C138 L139 D142 C143 D148 PHE SER ASP K152 N158 L159 G160 H161 Y162 V163 I164 K165 E166 K167 R168 L169 S170 T174 D180 R183 V184 A187 L188 H189 Q190

K191 N192 I193 L200 G201 N202 T215 N216 F217 H222 L229 D232 Q233 R234 G235 S236 P237 A238 Y239 I240 S241 P242 D243 R248 P249 Y250 D256 M257 W258 A259 L260 G261 V262 V263 M267 L268 Y269 I286 K287 A288 Y291 P294 E295 D296 G297 L310 L311 V312

L313 S329 W335 Q336 SER LEU SER

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.55Å 237.65Å 55.61Å 90.00° 106.32° 90.00°	Depositor
Resolution (Å)	59.41 – 2.53 59.41 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.6 (59.41-2.53) 98.6 (59.41-2.53)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	47.95 (at 2.55Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.258 , 0.280 0.266 , 0.288	Depositor DCC
R_{free} test set	2384 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	62.4	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 55.2	EDS
L-test for twinning[2]	$<|L|> = 0.45, <L^2> = 0.28$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8350	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.56	0/2208	0.54	0/3005
1	B	0.57	1/2114 (0.0%)	0.52	0/2882
1	C	0.35	0/2058	0.55	0/2810
1	D	0.44	0/2060	0.60	0/2828
All	All	0.49	1/8440 (0.0%)	0.55	0/11525

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	162	TYR	CE1-CZ	-5.10	1.31	1.38

There are no bond angle outliers.

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	2166	0	2083	55	0
1	B	2072	0	1932	55	0
1	C	2023	0	1873	45	0
1	D	2023	0	1718	59	0
2	A	20	0	0	2	0
2	B	17	0	0	2	0
2	C	16	0	0	0	0
2	D	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8350	0	7606	213	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 13.

All (213) 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:D:241:SER:CB	1:D:242:PRO:CD	2.19	1.16
1:B:303:THR:HG22	1:B:331:ILE:HD13	1.38	1.06
1:B:94:TYR:CE1	1:B:109:HIS:HE1	1.78	1.01
1:D:241:SER:CB	1:D:242:PRO:HD2	1.91	1.00
1:D:241:SER:CB	1:D:242:PRO:HD3	1.94	0.97
1:A:177:ILE:CG2	1:A:212:ILE:HD11	1.98	0.94
1:A:177:ILE:HG23	1:A:212:ILE:HD11	1.52	0.91
1:B:192:ASN:HB3	1:B:223:LEU:HB2	1.52	0.91
1:D:239:TYR:HD1	1:D:262:VAL:CG2	1.85	0.89
1:D:63:TYR:HA	1:D:143:CYS:HB2	1.55	0.87
1:A:229:LEU:HD21	1:A:249:PRO:HB3	1.55	0.86
1:B:331:ILE:O	1:B:334:SER:OG	1.94	0.84
1:B:67:ILE:HD12	1:B:138:CYS:SG	2.18	0.84
1:B:175:VAL:CG2	1:B:335:TRP:HH2	1.91	0.83
1:D:100:LEU:HD23	1:D:106:VAL:HG11	1.60	0.82
1:B:94:TYR:CE1	1:B:109:HIS:CE1	2.67	0.81
1:B:94:TYR:CD1	1:B:109:HIS:CE1	2.68	0.80
1:D:166:GLU:HB2	1:D:169:LEU:HD21	1.63	0.78
1:D:239:TYR:HD1	1:D:262:VAL:HG23	1.47	0.78
1:B:165:LYS:HD2	1:A:148:ASP:O	1.84	0.77
1:A:92:THR:O	1:A:96:LEU:HD12	1.84	0.77
1:B:303:THR:HG22	1:B:331:ILE:CD1	2.13	0.77
1:B:59:THR:HG23	1:B:61:ASP:H	1.51	0.76
1:B:94:TYR:CD1	1:B:109:HIS:HE1	2.05	0.75
1:C:53:LEU:HA	1:C:64:GLN:HA	1.69	0.74
1:A:67:ILE:HG12	1:A:138:CYS:HB3	1.70	0.74
1:B:309:LYS:HB3	1:B:319:LEU:HD13	1.70	0.73
1:D:239:TYR:CD1	1:D:262:VAL:CG2	2.72	0.73
1:B:225:SER:O	2:B:401:HOH:O	2.06	0.72
1:D:168:ARG:HG3	1:D:269:TYR:HA	1.70	0.72
1:B:175:VAL:HG21	1:B:335:TRP:CH2	2.24	0.71
1:B:266:THR:HG22	1:B:272:PHE:HA	1.72	0.71
1:D:239:TYR:CD1	1:D:262:VAL:HG23	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:ASP:O	1:D:250:TYR:OH	2.07	0.70
1:B:175:VAL:CG2	1:B:335:TRP:CH2	2.74	0.69
1:C:245:LEU:HB3	1:C:287:LYS:HE2	1.73	0.69
1:C:52:CYS:O	1:C:65:LEU:N	2.24	0.68
1:C:243:ASP:OD2	1:C:318:ARG:NH2	2.26	0.68
1:A:177:ILE:HG23	1:A:212:ILE:CD1	2.23	0.67
1:C:167:LYS:O	1:C:270:GLY:HA3	1.95	0.67
1:A:159:LEU:HG	1:A:200:LEU:HD23	1.76	0.67
1:A:59:THR:HG23	1:A:61:ASP:H	1.61	0.66
1:C:112:LEU:HD13	1:C:139:LEU:HD13	1.77	0.66
1:D:239:TYR:HD1	1:D:262:VAL:HG21	1.61	0.66
1:C:81:GLN:O	1:C:82:GLU:C	2.34	0.66
1:D:260:LEU:HA	1:D:263:VAL:HG12	1.80	0.64
1:A:285:LYS:HG3	1:A:290:GLU:HB3	1.79	0.63
1:D:55:ARG:NH2	2:D:401:HOH:O	2.30	0.63
1:B:147:HIS:HE1	1:B:150:SER:HB3	1.62	0.63
1:D:239:TYR:CD1	1:D:262:VAL:HG21	2.34	0.63
1:A:117:THR:O	1:A:134:LYS:N	2.29	0.62
1:C:66:LYS:NZ	1:C:216:ASN:ND2	2.47	0.62
1:A:312:VAL:O	1:A:318:ARG:NH2	2.30	0.62
1:D:115:ASP:OD2	1:D:136:ARG:NH2	2.32	0.62
1:D:50:VAL:HG13	1:D:67:ILE:HB	1.81	0.62
1:B:271:GLN:NE2	2:B:404:HOH:O	2.32	0.61
1:C:128:ARG:H	1:C:128:ARG:HD3	1.65	0.61
1:B:157:ILE:HB	1:B:207:LYS:HE2	1.82	0.61
1:A:31:ARG:NH2	1:A:57:ASP:OD2	2.34	0.60
1:D:166:GLU:CB	1:D:169:LEU:HD21	2.30	0.60
1:C:196:ARG:NH2	1:C:250:TYR:OH	2.34	0.60
1:A:328:LEU:HA	1:A:331:ILE:HD12	1.83	0.60
1:A:177:ILE:CG2	1:A:212:ILE:CD1	2.76	0.59
1:B:160:GLN:O	1:B:164:ILE:HG13	2.02	0.59
1:D:200:LEU:HG	1:D:263:VAL:HG23	1.83	0.59
1:D:35:PHE:HD2	1:D:65:LEU:HD11	1.68	0.59
1:C:69:THR:HA	1:C:136:ARG:HG2	1.85	0.58
1:C:112:LEU:HD12	1:C:138:CYS:O	2.04	0.58
1:C:263:VAL:O	1:C:267:MET:HG3	2.04	0.58
1:B:59:THR:HG23	1:B:61:ASP:N	2.19	0.58
1:D:161:HIS:O	1:D:164:ILE:HG12	2.04	0.57
1:A:169:LEU:HD22	1:A:173:GLU:OE2	2.05	0.56
1:C:81:GLN:O	1:C:84:ARG:N	2.38	0.56
1:D:55:ARG:NH1	1:D:59:THR:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LEU:HA	1:D:250:TYR:O	2.04	0.56
1:C:199:LYS:NZ	1:C:236:SER:OG	2.37	0.56
1:B:307:ILE:HG23	1:B:311:LEU:HD12	1.87	0.56
1:C:99:LEU:HD23	1:C:193:ILE:HD11	1.89	0.55
1:A:165:LYS:O	1:A:165:LYS:HG2	2.07	0.55
1:A:212:ILE:CG2	1:A:213:THR:N	2.70	0.55
1:C:178:PHE:O	1:C:181:VAL:HG22	2.07	0.55
1:B:53:LEU:HD12	1:B:54:ALA:H	1.71	0.55
1:A:68:LEU:HB2	1:A:90:LEU:HD11	1.89	0.54
1:A:64:GLN:NE2	2:A:401:HOH:O	2.28	0.54
1:C:269:TYR:CE2	1:C:293:ILE:HG23	2.42	0.54
1:D:239:TYR:O	1:D:258:TRP:CD1	2.60	0.54
1:B:310:LEU:O	1:B:318:ARG:HD3	2.08	0.54
1:B:171:GLU:HG3	1:B:299:VAL:HG23	1.90	0.54
1:B:54:ALA:HB3	1:B:65:LEU:HD13	1.90	0.54
1:C:281:GLU:O	1:C:285:LYS:HG3	2.08	0.54
1:A:69:THR:HA	1:A:136:ARG:HA	1.90	0.53
1:A:166:GLU:O	1:A:167:LYS:HB2	2.07	0.53
1:D:184:VAL:O	1:D:188:LEU:HD12	2.08	0.53
1:A:276:ASP:H	1:A:282:LEU:HD23	1.74	0.53
1:D:248:ARG:CB	1:D:249:PRO:CD	2.87	0.53
1:B:94:TYR:O	1:B:98:SER:OG	2.23	0.53
1:B:180:ASP:HA	1:B:183:ARG:HB3	1.90	0.52
1:D:93:GLU:OE2	1:D:217:PHE:N	2.42	0.52
1:D:187:ALA:O	1:D:191:LYS:HG3	2.09	0.52
1:A:118:CYS:HA	1:A:133:MET:HA	1.90	0.51
1:A:269:TYR:OH	1:A:299:VAL:HG11	2.11	0.51
1:A:68:LEU:HB2	1:A:90:LEU:CD1	2.41	0.51
1:C:64:GLN:HG2	1:C:142:ASP:O	2.10	0.51
1:C:100:LEU:O	1:C:108:HIS:ND1	2.42	0.51
1:C:181:VAL:HG12	1:C:212:ILE:HG12	1.92	0.51
1:B:170:SER:O	1:B:174:THR:OG1	2.24	0.51
1:C:178:PHE:O	1:C:182:VAL:HG23	2.11	0.51
1:B:196:ARG:NH2	1:B:234:ARG:O	2.43	0.50
1:B:100:LEU:HB3	1:B:103:GLN:HB3	1.92	0.50
1:C:100:LEU:HB3	1:C:103:GLN:HB3	1.94	0.50
1:A:97:LEU:HD22	1:A:107:VAL:O	2.12	0.50
1:A:80:SER:OG	1:A:81:GLN:N	2.44	0.50
1:A:189:HIS:HD2	1:A:321:ALA:HB2	1.76	0.50
1:A:234:ARG:NE	2:A:405:HOH:O	2.38	0.49
1:A:192:ASN:HB3	1:A:223:LEU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ASP:N	1:A:282:LEU:HD23	2.28	0.49
1:A:153:THR:HB	1:A:156:LEU:HD12	1.95	0.48
1:B:200:LEU:HD11	1:B:266:THR:OG1	2.13	0.48
1:A:55:ARG:NH1	1:A:59:THR:O	2.36	0.48
1:B:113:PHE:O	1:B:138:CYS:N	2.41	0.48
1:D:59:THR:OG1	1:D:60:ASP:N	2.45	0.48
1:A:212:ILE:HG22	1:A:213:THR:N	2.28	0.48
1:B:56:LYS:O	1:B:59:THR:HG22	2.14	0.48
1:D:269:TYR:CE1	1:D:294:PRO:HG2	2.48	0.48
1:B:262:VAL:O	1:B:266:THR:HG23	2.14	0.48
1:D:184:VAL:HG12	1:D:188:LEU:HD11	1.95	0.47
1:B:182:VAL:HG22	1:B:260:LEU:HD13	1.95	0.47
1:B:283:PHE:HB3	1:B:287:LYS:HE2	1.95	0.47
1:D:100:LEU:HD11	1:D:193:ILE:HD12	1.96	0.47
1:D:168:ARG:NH2	1:D:296:ASP:OD2	2.47	0.47
1:A:103:GLN:O	1:A:108:HIS:NE2	2.46	0.47
1:D:120:ILE:HA	1:D:131:LYS:HA	1.96	0.47
1:A:301:GLU:HA	1:A:304:VAL:HG22	1.94	0.47
1:A:306:LEU:HD13	1:A:324:VAL:HG23	1.96	0.47
1:D:104:ASP:OD1	1:D:183:ARG:NH1	2.48	0.47
1:D:163:VAL:O	1:D:167:LYS:N	2.48	0.46
1:D:170:SER:O	1:D:174:THR:HG23	2.15	0.46
1:D:158:ASN:OD1	1:D:160:GLN:N	2.47	0.46
1:A:94:TYR:HE1	1:A:109:HIS:CE1	2.34	0.46
1:C:99:LEU:HD21	1:C:222:HIS:ND1	2.31	0.46
1:A:54:ALA:HB3	1:A:65:LEU:HD13	1.97	0.46
1:B:159:LEU:O	1:B:163:VAL:HG13	2.16	0.46
1:B:97:LEU:HD22	1:B:107:VAL:O	2.15	0.46
1:D:250:TYR:CD1	1:D:250:TYR:N	2.84	0.46
1:A:80:SER:HB3	1:A:83:GLU:HG2	1.98	0.46
1:C:324:VAL:O	1:C:328:LEU:HD12	2.17	0.45
1:B:97:LEU:HD21	1:B:217:PHE:CD1	2.51	0.45
1:A:110:HIS:NE2	1:A:142:ASP:OD1	2.45	0.45
1:A:274:PHE:CE1	1:A:291:TYR:HB3	2.51	0.45
1:A:320:ALA:O	1:A:324:VAL:HG12	2.16	0.45
1:B:106:VAL:HG12	1:B:107:VAL:O	2.16	0.45
1:D:202:ASN:HB3	1:D:215:THR:O	2.17	0.45
1:A:68:LEU:CD2	1:A:68:LEU:C	2.85	0.45
1:C:243:ASP:HB3	1:C:250:TYR:HB2	1.99	0.45
1:A:185:VAL:HG11	1:A:260:LEU:HD11	1.97	0.44
1:B:50:VAL:HG23	1:B:67:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:PHE:CD2	1:D:65:LEU:HD11	2.48	0.44
1:D:168:ARG:HG3	1:D:268:LEU:O	2.18	0.44
1:D:158:ASN:HD21	1:D:201:GLY:HA2	1.82	0.44
1:B:293:ILE:HG13	1:B:293:ILE:O	2.17	0.44
1:C:54:ALA:O	1:C:63:TYR:N	2.51	0.44
1:B:175:VAL:HG21	1:B:335:TRP:CZ2	2.53	0.44
1:C:66:LYS:HZ3	1:C:216:ASN:ND2	2.16	0.44
1:D:54:ALA:HB3	1:D:65:LEU:HD12	1.99	0.44
1:A:104:ASP:CG	1:A:183:ARG:HH22	2.22	0.43
1:A:177:ILE:O	1:A:181:VAL:HG23	2.18	0.43
1:A:26:GLY:N	1:A:55:ARG:HH21	2.16	0.43
1:D:55:ARG:HA	1:D:62:PHE:HA	2.00	0.43
1:C:94:TYR:CE2	1:C:112:LEU:HD22	2.53	0.43
1:A:56:LYS:O	1:A:59:THR:HG22	2.19	0.43
1:B:34:PRO:O	1:B:56:LYS:HA	2.19	0.43
1:B:177:ILE:O	1:B:181:VAL:HG23	2.18	0.43
1:D:161:HIS:O	1:D:162:TYR:C	2.57	0.43
1:C:119:GLU:HG2	1:C:120:ILE:H	1.83	0.43
1:A:198:LEU:HD13	1:A:260:LEU:HD21	2.00	0.43
1:B:94:TYR:HE1	1:B:109:HIS:HE1	1.55	0.43
1:C:265:PHE:CG	1:C:273:PRO:HG3	2.53	0.43
1:D:32:ALA:H	1:D:37:LEU:HD13	1.84	0.43
1:C:48:SER:HB2	1:C:68:LEU:CD1	2.49	0.43
1:C:100:LEU:HD23	1:C:191:LYS:NZ	2.34	0.42
1:C:269:TYR:HE1	1:C:297:GLY:H	1.66	0.42
1:C:99:LEU:CD2	1:C:193:ILE:HD11	2.49	0.42
1:D:33:GLY:HA3	1:D:34:PRO:HD3	1.88	0.42
1:A:262:VAL:HG13	1:A:273:PRO:HD2	2.01	0.42
1:D:68:LEU:HD21	1:D:87:LYS:HA	2.00	0.42
1:B:147:HIS:CE1	1:B:150:SER:HB3	2.49	0.42
1:D:37:LEU:HG	1:D:52:CYS:SG	2.60	0.42
1:C:307:ILE:O	1:C:311:LEU:HG	2.20	0.42
1:D:96:LEU:HD22	1:D:222:HIS:HB2	2.02	0.42
1:C:66:LYS:HZ1	1:C:216:ASN:ND2	2.15	0.41
1:C:50:VAL:O	1:C:67:ILE:HG22	2.18	0.41
1:D:107:VAL:HG23	1:D:142:ASP:HB2	2.02	0.41
1:C:278:ILE:CG2	1:C:281:GLU:HB3	2.50	0.41
1:D:99:LEU:HD11	1:D:222:HIS:CD2	2.54	0.41
1:D:236:SER:HA	1:D:237:PRO:HD3	1.72	0.41
1:A:56:LYS:HB3	1:A:59:THR:CG2	2.51	0.41
1:C:46:VAL:HG12	1:C:47:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLN:HA	1:C:84:ARG:HB2	2.02	0.41
1:A:170:SER:O	1:A:174:THR:OG1	2.14	0.41
1:B:199:LYS:HE2	1:B:236:SER:OG	2.21	0.41
1:B:300:SER:O	1:B:304:VAL:HG23	2.21	0.41
1:D:174:THR:HG21	1:D:268:LEU:HD23	2.03	0.41
1:B:258:TRP:HB2	1:B:318:ARG:NH1	2.36	0.41
1:C:161:HIS:HA	1:C:164:ILE:HG12	2.03	0.41
1:D:180:ASP:O	1:D:184:VAL:HG23	2.21	0.41
1:C:293:ILE:HA	1:C:294:PRO:HD3	1.83	0.40
1:C:89:LEU:HA	1:C:89:LEU:HD23	1.89	0.40
1:D:50:VAL:O	1:D:67:ILE:N	2.50	0.40
1:B:94:TYR:HE1	1:B:109:HIS:CE1	2.34	0.40
1:B:172:ARG:HD3	1:B:172:ARG:HH11	1.74	0.40
1:B:35:PHE:HB3	1:B:54:ALA:HB1	2.03	0.40
1:D:263:VAL:O	1:D:267:MET:HG3	2.22	0.40
1:A:104:ASP:OD1	1:A:183:ARG:NH2	2.54	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	285/320 (89%)	271 (95%)	14 (5%)	0	100	100
1	B	276/320 (86%)	264 (96%)	12 (4%)	0	100	100
1	C	275/320 (86%)	259 (94%)	16 (6%)	0	100	100
1	D	288/320 (90%)	260 (90%)	28 (10%)	0	100	100
All	All	1124/1280 (88%)	1054 (94%)	70 (6%)	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	215/283 (76%)	208 (97%)	7 (3%)	45	71
1	B	204/283 (72%)	201 (98%)	3 (2%)	72	90
1	C	188/283 (66%)	184 (98%)	4 (2%)	61	84
1	D	172/283 (61%)	161 (94%)	11 (6%)	22	38
All	All	779/1132 (69%)	754 (97%)	25 (3%)	46	73

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	64	GLN
1	C	128	ARG
1	C	190	GLN
1	C	275	TYR
1	B	109	HIS
1	B	172	ARG
1	B	329	SER
1	A	68	LEU
1	A	96	LEU
1	A	99	LEU
1	A	183	ARG
1	A	225	SER
1	A	230	LEU
1	A	296	ASP
1	D	63	TYR
1	D	64	GLN
1	D	65	LEU
1	D	89	LEU
1	D	161	HIS
1	D	183	ARG
1	D	189	HIS
1	D	234	ARG
1	D	243	ASP
1	D	256	ASP
1	D	329	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	GLN
1	C	216	ASN
1	B	109	HIS
1	B	147	HIS
1	B	190	GLN
1	A	161	HIS
1	A	189	HIS
1	A	216	ASN
1	D	192	ASN
1	D	222	HIS

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 carbohydrates 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 (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, 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(Å²)	Q<0.9
1	A	293/320 (91%)	-0.01	3 (1%)	84	86	39, 68, 107, 145	0
1	B	282/320 (88%)	0.15	6 (2%)	67	71	39, 71, 125, 171	0
1	C	282/320 (88%)	0.44	24 (8%)	13	14	39, 86, 144, 189	0
1	D	294/320 (91%)	0.34	21 (7%)	19	21	64, 102, 137, 166	0
All	All	1151/1280 (89%)	0.23	54 (4%)	35	40	39, 83, 134, 189	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	149	PHE	4.8
1	C	112	LEU	4.7
1	C	137	ILE	4.5
1	B	118	CYS	4.3
1	C	306	LEU	4.2
1	D	291	TYR	4.2
1	D	235	GLY	4.0
1	D	310	LEU	3.8
1	C	113	PHE	3.8
1	C	135	LYS	3.6
1	C	54	ALA	3.6
1	D	297	GLY	3.5
1	D	130	VAL	3.5
1	D	118	CYS	3.3
1	C	148	ASP	3.3
1	B	279	PRO	3.3
1	D	288	ALA	3.3
1	D	121	VAL	3.3
1	D	133	MET	3.1
1	C	115	ASP	3.0
1	C	312	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	138	CYS	2.9
1	D	126	SER	2.9
1	A	78	ILE	2.9
1	C	69	THR	2.8
1	B	229	LEU	2.8
1	C	121	VAL	2.8
1	C	52	CYS	2.6
1	D	335	TRP	2.6
1	B	223	LEU	2.5
1	C	278	ILE	2.5
1	D	132	LYS	2.5
1	D	162	TYR	2.4
1	C	114	GLN	2.4
1	D	119	GLU	2.3
1	C	53	LEU	2.3
1	A	312	VAL	2.3
1	C	288	ALA	2.3
1	D	286	ILE	2.2
1	C	131	LYS	2.2
1	D	120	ILE	2.2
1	D	139	LEU	2.2
1	C	127	SER	2.2
1	D	311	LEU	2.2
1	D	137	ILE	2.2
1	C	308	ARG	2.1
1	D	129	MET	2.1
1	C	315	PRO	2.1
1	C	136	ARG	2.1
1	B	228	ASP	2.1
1	A	90	LEU	2.1
1	C	310	LEU	2.1
1	D	313	LEU	2.0
1	C	147	HIS	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.