Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 01:35 PM EDT

PDB ID	:	9CB5 / pdb_00009cb5
Title	:	Crystal structure of nucleolin in complex with MYC promoter G-quadruplex
Authors	:	Chen, L.; Dickerhoff, J.; Noinaj, N.; Yang, D.
Deposited on	:	2024-06-18
Resolution	:	2.60 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:

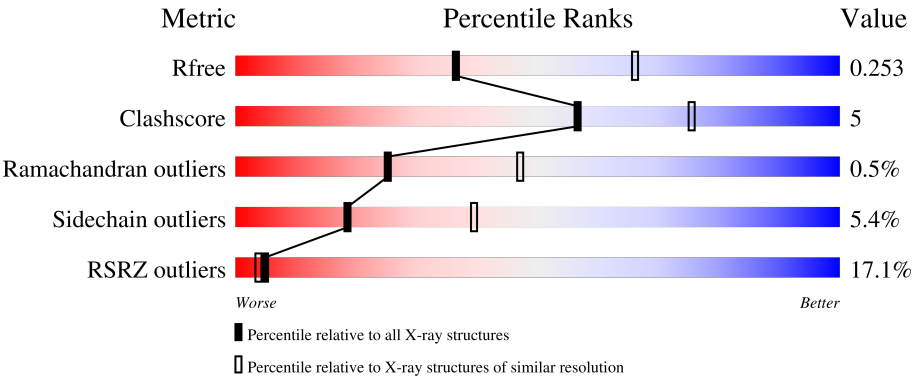
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.60 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	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	347	22% 43% 5% 51%
1	B	347	% 44% 5% 51%
2	C	28	4% 86% 14%
2	F	28	18% 64% 14% 18%
3	D	246	7% 85% 10% 5%

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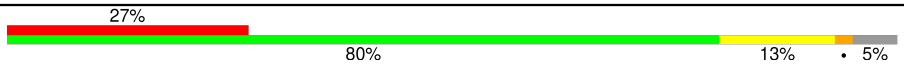
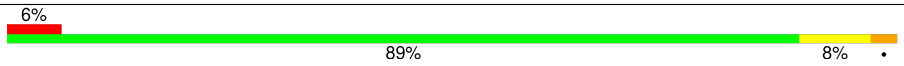
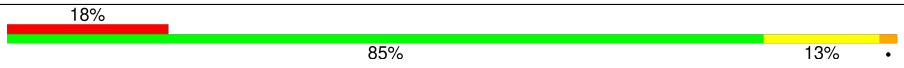
Mol	Chain	Length	Quality of chain
3	G	246	
4	H	215	
4	I	215	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10339 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 Nucleolin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	1	0
			1106	687	201	216	2			
1	B	171	Total	C	N	O	S	0	0	0
			1342	848	225	267	2			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	301	GLY	-	expression tag	UNP P19338
A	302	GLY	-	expression tag	UNP P19338
A	303	GLY	-	expression tag	UNP P19338
A	304	GLY	-	expression tag	UNP P19338
A	305	HIS	-	expression tag	UNP P19338
A	306	MET	-	expression tag	UNP P19338
A	543	SER	CYS	conflict	UNP P19338
B	301	GLY	-	expression tag	UNP P19338
B	302	GLY	-	expression tag	UNP P19338
B	303	GLY	-	expression tag	UNP P19338
B	304	GLY	-	expression tag	UNP P19338
B	305	HIS	-	expression tag	UNP P19338
B	306	MET	-	expression tag	UNP P19338
B	543	SER	CYS	conflict	UNP P19338

- Molecule 2 is a DNA chain called MYC promoter G-quadruplex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	28	Total	C	N	O	P	0	0	0
			585	278	109	171	27			
2	F	23	Total	C	N	O	P	0	0	0
			487	230	91	143	23			

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	234	Total	C	N	O	S	0	0	0
			1749	1114	289	340	6			
3	G	233	Total	C	N	O	S	0	0	0
			1712	1089	284	332	7			

- Molecule 4 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	215	Total	C	N	O	S	0	0	0
			1597	994	269	328	6			
4	I	215	Total	C	N	O	S	0	0	0
			1568	972	266	324	6			

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	K	0	0
			2	2		
5	F	2	Total	K	0	0
			2	2		

- Molecule 6 is water.

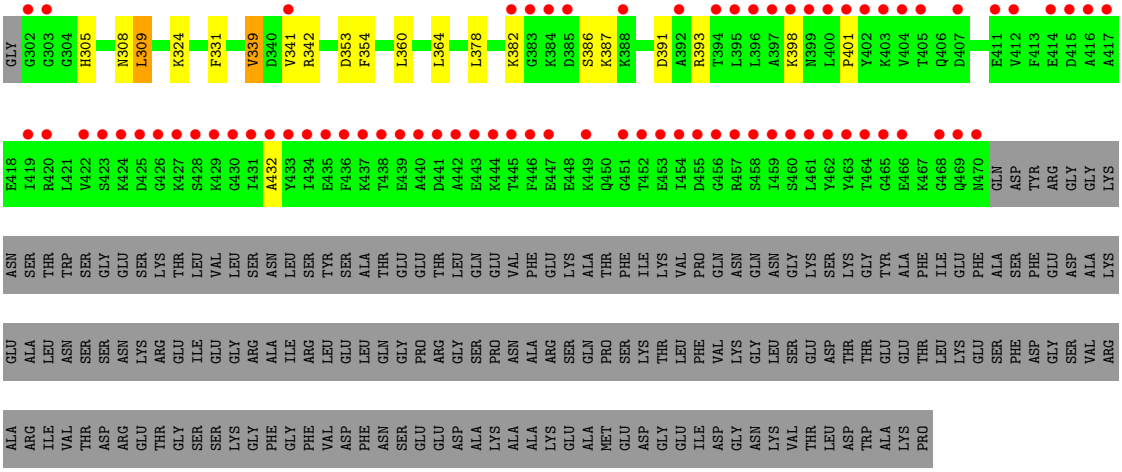
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	34	Total	O	0	0
			34	34		
6	C	12	Total	O	0	0
			12	12		
6	D	35	Total	O	0	0
			35	35		
6	F	5	Total	O	0	0
			5	5		
6	G	21	Total	O	0	0
			21	21		
6	H	55	Total	O	0	0
			55	55		
6	I	20	Total	O	0	0
			20	20		

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.

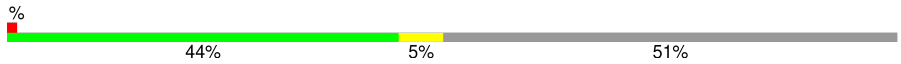
• Molecule 1: Nucleolin

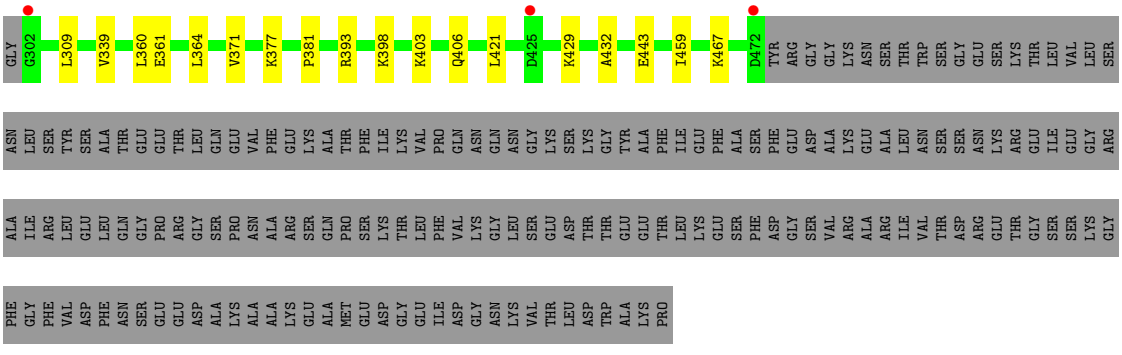
Chain A:



• Molecule 1: Nucleolin

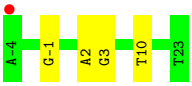
Chain B:





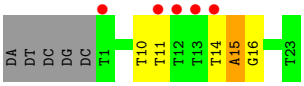
• Molecule 2: MYC promoter G-quadruplex

Chain C:



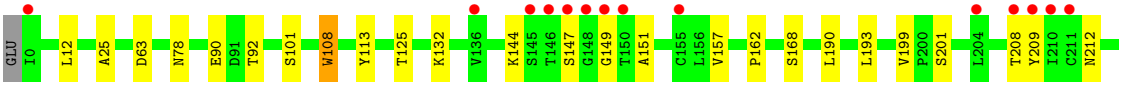
• Molecule 2: MYC promoter G-quadruplex

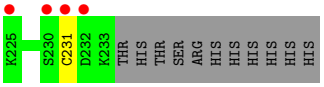
Chain F:



• Molecule 3: Fab heavy chain

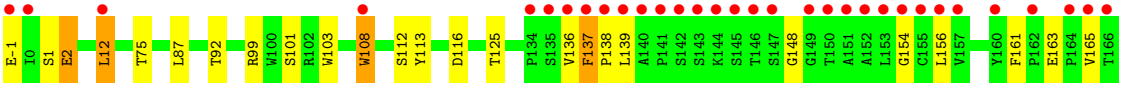
Chain D:

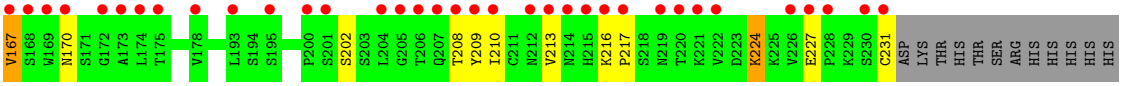




• Molecule 3: Fab heavy chain

Chain G:



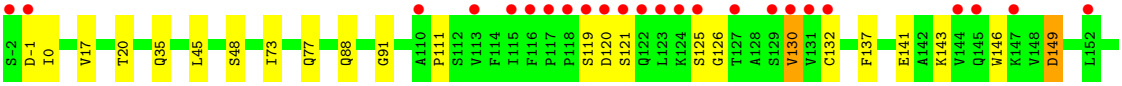


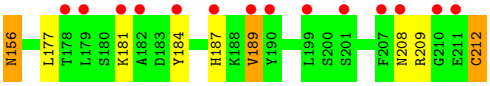
• Molecule 4: Fab light chain

Chain H:

• Molecule 4: Fab light chain

Chain I:




N156
L177
T178
L179
S180
K181
A182
D183
Y184
H187
K188
V189
Y190
L199
S200
S201
F207
N208
R209
G210
E211
C212

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.25Å 134.66Å 185.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.43 – 2.60 48.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.43-2.60) 96.7 (48.43-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.21.1_5286: ???)	Depositor
R, R_{free}	0.232 , 0.254 0.232 , 0.253	Depositor DCC
R_{free} test set	56399 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10339	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

Bond lengths and bond angles in the following residue types are not validated in this section: K

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	0.26	0/1117	0.48	0/1514
1	B	0.25	0/1360	0.45	0/1818
2	C	0.49	0/657	0.90	0/1017
2	F	0.54	0/547	0.99	1/847 (0.1%)
3	D	0.25	0/1799	0.50	0/2460
3	G	0.26	0/1761	0.50	0/2408
4	H	0.25	0/1630	0.49	0/2216
4	I	0.27	0/1600	0.50	0/2179
All	All	0.30	0/10471	0.57	1/14459 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	15	DA	O4'-C1'-N9	5.32	111.73	108.00

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	1106	0	906	16	0
1	B	1342	0	1342	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	585	0	319	3	0
2	F	487	0	262	6	0
3	D	1749	0	1652	12	0
3	G	1712	0	1578	28	0
4	H	1597	0	1532	10	0
4	I	1568	0	1458	19	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
6	A	7	0	0	0	0
6	B	34	0	0	0	0
6	C	12	0	0	0	0
6	D	35	0	0	0	0
6	F	5	0	0	0	0
6	G	21	0	0	0	0
6	H	55	0	0	0	0
6	I	20	0	0	0	0
All	All	10339	0	9049	86	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 5.

All (86) 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)
3:G:231:CYS:SG	4:I:212:CYS:N	2.46	0.87
1:A:342:ARG:NH2	2:F:10:DT:O4	2.19	0.75
1:A:309:LEU:HD21	1:A:364:LEU:HG	1.72	0.70
1:A:308:ASN:HD21	2:F:10:DT:H3	1.40	0.69
1:A:324:LYS:HA	1:A:341:VAL:HG11	1.75	0.68
3:G:101:SER:HB2	3:G:113:TYR:HB3	1.76	0.67
3:G:101:SER:HA	3:G:116:ASP:HB2	1.77	0.67
3:D:132:LYS:HD3	3:D:190:LEU:HD21	1.78	0.65
4:I:111:PRO:HA	4:I:137:PHE:HB3	1.77	0.64
1:A:309:LEU:HB2	1:A:354:PHE:HE2	1.63	0.63
3:G:138:PRO:HB3	4:I:119:SER:HB2	1.80	0.62
4:H:116:PHE:HB2	4:H:131:VAL:HG23	1.80	0.61
4:I:184:TYR:O	4:I:209:ARG:NH2	2.34	0.60
2:F:15:DA:H2"	2:F:16:DG:C8	2.37	0.59
4:I:130:VAL:HG13	4:I:177:LEU:HB3	1.85	0.59
3:G:216:LYS:HB3	3:G:217:PRO:HD3	1.86	0.58
1:A:339:VAL:HA	3:G:1:SER:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:92:THR:HG23	3:D:125:THR:HA	1.86	0.57
3:D:147:SER:O	3:D:149:GLY:N	2.38	0.54
1:A:305[A]:HIS:ND1	3:G:75:THR:OG1	2.36	0.54
1:B:443:GLU:OE2	1:B:467:LYS:NZ	2.39	0.54
1:B:421:LEU:HD23	1:B:432:ALA:HB2	1.90	0.53
4:H:162:THR:HG22	4:H:172:SER:H	1.74	0.53
3:G:99:ARG:NH2	3:G:116:ASP:OD2	2.42	0.53
1:B:309:LEU:HD11	1:B:364:LEU:HG	1.90	0.53
4:H:27:VAL:HG11	4:H:88:GLN:HG3	1.91	0.52
4:I:119:SER:O	4:I:121:SER:N	2.41	0.52
4:H:148:VAL:HG22	4:H:151:ALA:HB3	1.90	0.52
3:G:92:THR:HG23	3:G:125:THR:HA	1.92	0.52
3:D:168:SER:HB3	3:D:212:ASN:HB2	1.92	0.51
3:G:137:PHE:HB2	3:G:138:PRO:HD3	1.93	0.51
1:A:308:ASN:ND2	2:F:10:DT:H3	2.08	0.50
2:F:14:DT:H3	2:F:15:DA:H2	1.59	0.50
4:I:156:ASN:OD1	4:I:156:ASN:N	2.45	0.49
3:G:137:PHE:HB3	4:I:119:SER:HB3	1.94	0.49
4:I:35:GLN:HB2	4:I:45:LEU:HD11	1.93	0.49
3:G:138:PRO:HD3	3:G:156:LEU:HB3	1.96	0.48
3:D:157:VAL:HB	3:D:193:LEU:HB3	1.95	0.48
3:G:231:CYS:HB2	4:I:212:CYS:OXT	2.14	0.48
2:C:2:DA:H2"	2:C:3:DG:C8	2.49	0.47
3:G:137:PHE:CB	3:G:138:PRO:HD3	2.44	0.47
3:G:2:GLU:OE1	3:G:2:GLU:N	2.45	0.47
3:G:167:VAL:HG23	3:G:213:VAL:HA	1.97	0.47
4:I:121:SER:O	4:I:125:SER:N	2.49	0.46
1:B:398:LYS:NZ	2:C:-1:DG:OP2	2.48	0.46
1:B:403:LYS:HA	1:B:403:LYS:HD3	1.71	0.45
3:G:139:LEU:HA	3:G:154:GLY:O	2.15	0.45
4:I:0:ILE:HD12	4:I:91:GLY:HA3	1.98	0.45
4:I:17:VAL:HG22	4:I:73:ILE:HB	1.97	0.45
1:A:386:SER:OG	1:A:387:LYS:N	2.49	0.45
1:A:382:LYS:O	2:F:11:DT:H5'	2.17	0.44
4:I:119:SER:C	4:I:121:SER:H	2.21	0.44
3:D:199:VAL:HG21	3:D:209:TYR:CE2	2.53	0.44
3:D:12:LEU:HD11	3:D:162:PRO:HG3	1.99	0.44
3:G:108:TRP:HA	3:G:108:TRP:CE3	2.52	0.44
3:D:144:LYS:H	3:D:144:LYS:HG3	1.60	0.44
1:A:331:PHE:HZ	1:A:378:LEU:HD21	1.82	0.44
3:D:151:ALA:HB2	3:D:201:SER:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:SER:OG	3:D:113:TYR:HB3	2.17	0.43
3:G:112:SER:OG	4:I:48:SER:OG	2.25	0.43
3:G:170:ASN:HB3	3:G:210:ILE:HG12	2.00	0.43
3:G:138:PRO:CB	4:I:119:SER:HB2	2.47	0.43
1:A:342:ARG:NH1	1:A:353:ASP:OD1	2.52	0.43
1:A:342:ARG:HG2	3:G:103:TRP:CG	2.53	0.43
4:H:125:SER:O	4:H:181:LYS:HD3	2.19	0.43
4:H:145:GLN:HG2	4:H:152:LEU:HD21	2.00	0.43
3:G:170:ASN:ND2	3:G:209:TYR:H	2.15	0.43
4:I:132:CYS:HB2	4:I:146:TRP:CH2	2.54	0.43
1:B:309:LEU:HD13	1:B:360:LEU:HG	2.00	0.43
4:I:126:GLY:HA2	4:I:181:LYS:HE2	2.00	0.43
1:A:398:LYS:HA	1:A:432:ALA:H	1.83	0.42
1:A:309:LEU:HD13	1:A:360:LEU:HD11	2.01	0.42
4:H:162:THR:HG23	4:H:163:GLU:O	2.18	0.42
3:G:148:GLY:HA2	3:G:202:SER:N	2.35	0.42
4:H:130:VAL:HB	4:H:177:LEU:HB3	2.02	0.42
3:D:108:TRP:HA	3:D:108:TRP:CE3	2.55	0.42
4:I:149:ASP:HA	4:I:189:VAL:HG12	2.02	0.41
3:D:25:ALA:O	3:D:78:ASN:ND2	2.51	0.41
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.87	0.41
1:B:381:PRO:HB2	2:C:10:DT:C2	2.56	0.41
3:G:170:ASN:N	3:G:210:ILE:O	2.53	0.41
3:G:108:TRP:HA	3:G:108:TRP:HE3	1.85	0.41
3:G:224:LYS:HE2	3:G:224:LYS:HB3	1.64	0.41
4:H:149:ASP:HA	4:H:189:VAL:HG13	2.01	0.41
3:G:12:LEU:HD11	3:G:161:PHE:HE2	1.85	0.40
4:H:98:GLN:OE1	4:H:98:GLN:N	2.46	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	168/347 (48%)	147 (88%)	20 (12%)	1 (1%)	22 43
1	B	169/347 (49%)	168 (99%)	1 (1%)	0	100 100
3	D	232/246 (94%)	219 (94%)	12 (5%)	1 (0%)	30 52
3	G	231/246 (94%)	208 (90%)	21 (9%)	2 (1%)	14 31
4	H	213/215 (99%)	201 (94%)	11 (5%)	1 (0%)	25 47
4	I	213/215 (99%)	193 (91%)	19 (9%)	1 (0%)	25 47
All	All	1226/1616 (76%)	1136 (93%)	84 (7%)	6 (0%)	25 47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	PRO
3	D	231	CYS
3	G	137	PHE
3	G	208	THR
4	H	149	ASP
4	I	189	VAL

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	78/289 (27%)	74 (95%)	4 (5%)	20 42
1	B	142/289 (49%)	134 (94%)	8 (6%)	17 38
3	D	185/208 (89%)	181 (98%)	4 (2%)	47 72
3	G	174/208 (84%)	163 (94%)	11 (6%)	15 32
4	H	180/187 (96%)	170 (94%)	10 (6%)	17 38
4	I	169/187 (90%)	156 (92%)	13 (8%)	10 22
All	All	928/1368 (68%)	878 (95%)	50 (5%)	18 39

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	LEU
1	A	339	VAL
1	A	391	ASP
1	A	393	ARG
1	B	339	VAL
1	B	361	GLU
1	B	371	VAL
1	B	377	LYS
1	B	393	ARG
1	B	406	GLN
1	B	429	LYS
1	B	459	ILE
3	D	63	ASP
3	D	90	GLU
3	D	108	TRP
3	D	208	THR
3	G	-1	GLU
3	G	2	GLU
3	G	12	LEU
3	G	87	LEU
3	G	108	TRP
3	G	136	VAL
3	G	163	GLU
3	G	165	VAL
3	G	167	VAL
3	G	224	LYS
3	G	227	GLU
4	H	-1	ASP
4	H	72	THR
4	H	120	ASP
4	H	131	VAL
4	H	145	GLN
4	H	148	VAL
4	H	152	LEU
4	H	162	THR
4	H	178	THR
4	H	203	VAL
4	I	-1	ASP
4	I	20	THR
4	I	77	GLN
4	I	88	GLN
4	I	120	ASP
4	I	130	VAL

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Mol	Chain	Res	Type
4	I	141	GLU
4	I	143	LYS
4	I	149	ASP
4	I	156	ASN
4	I	187	HIS
4	I	208	ASN
4	I	212	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	169/347 (48%)	1.77	76 (44%) 1 1	31, 106, 144, 151	1 (0%)
1	B	171/347 (49%)	0.07	3 (1%) 67 62	33, 49, 72, 83	0
2	C	28/28 (100%)	-0.09	1 (3%) 46 40	35, 48, 70, 112	0
2	F	23/28 (82%)	0.56	5 (21%) 3 2	51, 60, 128, 148	0
3	D	234/246 (95%)	0.43	18 (7%) 21 17	30, 50, 111, 134	0
3	G	233/246 (94%)	1.06	67 (28%) 1 1	38, 62, 140, 153	0
4	H	215/215 (100%)	0.27	12 (5%) 31 25	30, 47, 95, 119	0
4	I	215/215 (100%)	0.95	38 (17%) 4 3	39, 70, 127, 153	0
All	All	1288/1672 (77%)	0.72	220 (17%) 5 4	30, 58, 134, 153	1 (0%)

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	145	SER	5.9
2	C	-4	DA	5.8
3	G	209	TYR	5.6
3	G	138	PRO	5.5
1	A	458	SER	5.3
1	A	465	GLY	5.3
1	A	425	ASP	5.3
1	A	470	ASN	5.2
1	A	433	TYR	5.2
1	A	460	SER	5.0
1	A	427	LYS	4.9
1	A	423	SER	4.9
1	A	469	GLN	4.8
1	A	455	ASP	4.8
1	A	428	SER	4.7
3	G	140	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
4	I	118	PRO	4.7
1	A	397	ALA	4.6
1	A	459	ILE	4.6
1	A	464	THR	4.6
1	A	402	TYR	4.6
3	G	222	VAL	4.5
1	A	441	ASP	4.5
1	A	405	THR	4.5
4	I	117	PRO	4.4
3	G	153	LEU	4.4
1	A	400	LEU	4.4
3	G	220	THR	4.3
3	G	217	PRO	4.3
4	I	127	THR	4.3
1	A	424	LYS	4.2
1	A	466	GLU	4.1
4	I	131	VAL	4.1
3	D	0	ILE	4.1
3	G	0	ILE	4.1
1	A	415	ASP	4.1
3	D	225	LYS	4.0
3	G	139	LEU	4.0
1	B	472	ASP	4.0
1	A	431	ILE	4.0
3	G	195	SER	4.0
4	I	120	ASP	4.0
1	A	462	TYR	3.9
1	A	447	GLU	3.9
1	A	392	ALA	3.9
1	A	414	GLU	3.9
3	G	152	ALA	3.9
3	D	209	TYR	3.9
1	A	461	LEU	3.8
1	A	443	GLU	3.8
3	D	232	ASP	3.8
1	A	452	THR	3.8
3	G	208	THR	3.8
3	G	172	GLY	3.8
4	I	-2	SER	3.7
4	I	189	VAL	3.7
3	D	231	CYS	3.7
4	I	211	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	463	TYR	3.7
4	I	129	SER	3.7
3	D	146	THR	3.6
4	I	207	PHE	3.6
3	D	147	SER	3.6
1	A	457	ARG	3.6
3	G	219	ASN	3.6
1	A	438	THR	3.6
4	I	122	GLN	3.5
1	A	439	GLU	3.5
1	A	399	ASN	3.5
3	G	146	THR	3.5
1	A	456	GLY	3.4
3	D	148	GLY	3.4
1	A	403	LYS	3.4
3	G	149	GLY	3.4
1	A	416	ALA	3.3
4	I	116	PHE	3.3
3	G	108	TRP	3.3
3	G	165	VAL	3.3
1	A	440	ALA	3.3
3	G	166	THR	3.3
3	G	151	ALA	3.3
1	A	341	VAL	3.3
3	G	142	SER	3.2
3	G	231	CYS	3.2
1	A	430	GLY	3.2
1	A	446	PHE	3.2
4	I	178	THR	3.2
3	G	230	SER	3.2
1	A	412	VAL	3.2
1	A	454	ILE	3.1
4	H	149	ASP	3.1
3	G	164	PRO	3.1
1	A	407	ASP	3.1
3	D	149	GLY	3.1
4	I	184	TYR	3.1
1	A	302	GLY	3.1
3	G	150	THR	3.0
3	G	204	LEU	3.0
3	G	212	ASN	3.0
3	G	145	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	429	LYS	3.0
3	G	-1	GLU	3.0
1	B	425	ASP	3.0
3	D	150	THR	3.0
3	G	207	GLN	3.0
3	G	137	PHE	3.0
3	G	200	PRO	3.0
3	G	210	ILE	3.0
1	A	437	LYS	3.0
4	I	123	LEU	2.9
4	H	182	ALA	2.9
1	A	434	ILE	2.9
1	A	426	GLY	2.9
1	A	411	GLU	2.9
1	A	394	THR	2.9
1	A	453	GLU	2.9
4	H	112	SER	2.9
3	G	213	VAL	2.9
3	G	173	ALA	2.9
1	A	395	LEU	2.9
3	G	167	VAL	2.8
1	A	442	ALA	2.8
1	A	436	PHE	2.8
3	G	221	LYS	2.8
1	A	435	GLU	2.8
2	F	12	DT	2.8
3	G	134	PRO	2.8
3	G	155	CYS	2.7
3	D	230	SER	2.7
3	G	135	SER	2.7
3	G	175	THR	2.7
1	A	449	LYS	2.7
3	G	156	LEU	2.7
3	G	174	LEU	2.7
3	G	206	THR	2.7
2	F	1	DT	2.7
3	G	227	GLU	2.7
1	A	384	LYS	2.7
1	A	420	ARG	2.7
3	G	169	TRP	2.7
3	G	201	SER	2.7
1	A	404	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	422	VAL	2.6
2	F	11	DT	2.6
4	H	190	TYR	2.6
1	A	398	LYS	2.6
1	A	444	LYS	2.6
3	G	214	ASN	2.6
4	I	113	VAL	2.6
4	I	132	CYS	2.6
3	G	160	TYR	2.6
3	G	170	ASN	2.6
3	G	168	SER	2.6
4	H	-2	SER	2.6
3	G	144	LYS	2.5
2	F	14	DT	2.5
3	G	228	PRO	2.5
3	G	147	SER	2.5
4	I	125	SER	2.5
4	H	179	LEU	2.5
3	G	193	LEU	2.5
3	D	136	VAL	2.5
4	H	208	ASN	2.5
1	A	383	GLY	2.5
4	I	119	SER	2.5
2	F	13	DT	2.5
3	G	136	VAL	2.4
4	I	190	TYR	2.4
4	I	208	ASN	2.4
3	D	210	ILE	2.4
1	A	396	LEU	2.4
4	H	191	ALA	2.4
4	I	182	ALA	2.4
4	I	152	LEU	2.3
4	I	124	LYS	2.3
1	A	401	PRO	2.3
4	I	201	SER	2.3
4	I	130	VAL	2.3
3	G	12	LEU	2.3
4	I	115	ILE	2.3
1	A	417	ALA	2.3
1	A	382	LYS	2.3
3	D	208	THR	2.3
4	I	145	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
3	G	205	GLY	2.3
4	I	199	LEU	2.3
1	A	385	ASP	2.2
3	G	141	PRO	2.2
3	G	162	PRO	2.2
1	A	419	ILE	2.2
3	G	154	GLY	2.2
4	I	210	GLY	2.2
4	I	187	HIS	2.2
1	A	451	GLY	2.2
1	A	468	GLY	2.2
3	G	178	VAL	2.2
4	I	144	VAL	2.2
4	H	212	CYS	2.2
1	B	302	GLY	2.2
1	A	445	THR	2.2
3	G	157	VAL	2.2
1	A	432	ALA	2.2
4	H	185	GLU	2.1
4	H	154	SER	2.1
1	A	388	LYS	2.1
3	D	211	CYS	2.1
1	A	303	GLY	2.1
3	G	216	LYS	2.1
4	I	147	LYS	2.1
4	I	179	LEU	2.1
4	I	110	ALA	2.1
3	G	215	HIS	2.1
4	I	181	LYS	2.1
4	H	152	LEU	2.1
3	D	155	CYS	2.1
3	G	143	SER	2.1
3	G	226	VAL	2.1
3	D	204	LEU	2.0
4	I	121	SER	2.0
4	I	-1	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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
5	K	F	101	1/1	0.91	0.06	56,56,56,56	0
5	K	F	102	1/1	0.97	0.03	41,41,41,41	0
5	K	C	101	1/1	0.99	0.02	35,35,35,35	0
5	K	C	102	1/1	0.99	0.05	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.