Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 01:48 AM EDT

PDB ID	:	5DS5
Title	:	Crystal structure the Escherichia coli Cas1-Cas2 complex bound to protospacer DNA and Mg
Authors	:	Nunez, J.K.; Harrington, L.B.; Kranzusch, P.J.; Engelman, A.N.; Doudna, J.A.
Deposited on	:	2015-09-16
Resolution	:	2.95 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:

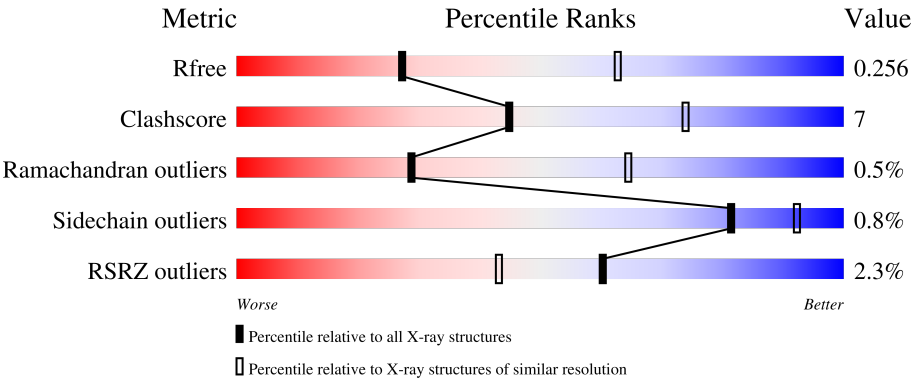
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	306	4% 68% 13% 18%
1	B	306	74% 16% 9%
1	C	306	3% 73% 9% 18%
1	D	306	3% 74% 15% • 10%
2	E	104	% 71% 19% 10%

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Mol	Chain	Length	Quality of chain
2	F	104	72% 17% 10%
3	G	28	50% 50%
4	H	28	82% 18%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10719 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 CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1907	1218	337	345	7			
1	B	277	Total	C	N	O	S	0	0	0
			2136	1367	379	383	7			
1	C	252	Total	C	N	O	S	0	0	0
			1926	1230	342	347	7			
1	D	275	Total	C	N	O	S	0	0	0
			2125	1362	377	379	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q46896
B	0	SER	-	expression tag	UNP Q46896
C	0	SER	-	expression tag	UNP Q46896
D	0	SER	-	expression tag	UNP Q46896

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	94	Total	C	N	O	S	0	0	0
			739	475	128	132	4			
2	F	94	Total	C	N	O	S	0	0	0
			739	475	128	132	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP P45956
E	95	GLY	-	expression tag	UNP P45956
E	96	SER	-	expression tag	UNP P45956
E	97	SER	-	expression tag	UNP P45956

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Chain	Residue	Modelled	Actual	Comment	Reference
E	98	GLU	-	expression tag	UNP P45956
E	99	ASN	-	expression tag	UNP P45956
E	100	LEU	-	expression tag	UNP P45956
E	101	TYR	-	expression tag	UNP P45956
E	102	PHE	-	expression tag	UNP P45956
E	103	GLN	-	expression tag	UNP P45956
F	0	MET	-	initiating methionine	UNP P45956
F	95	GLY	-	expression tag	UNP P45956
F	96	SER	-	expression tag	UNP P45956
F	97	SER	-	expression tag	UNP P45956
F	98	GLU	-	expression tag	UNP P45956
F	99	ASN	-	expression tag	UNP P45956
F	100	LEU	-	expression tag	UNP P45956
F	101	TYR	-	expression tag	UNP P45956
F	102	PHE	-	expression tag	UNP P45956
F	103	GLN	-	expression tag	UNP P45956

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	28	Total	C	N	O	P	0	0	0
			578	275	118	158	27			

- Molecule 4 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	28	Total	C	N	O	P	0	0	0
			564	274	86	177	27			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

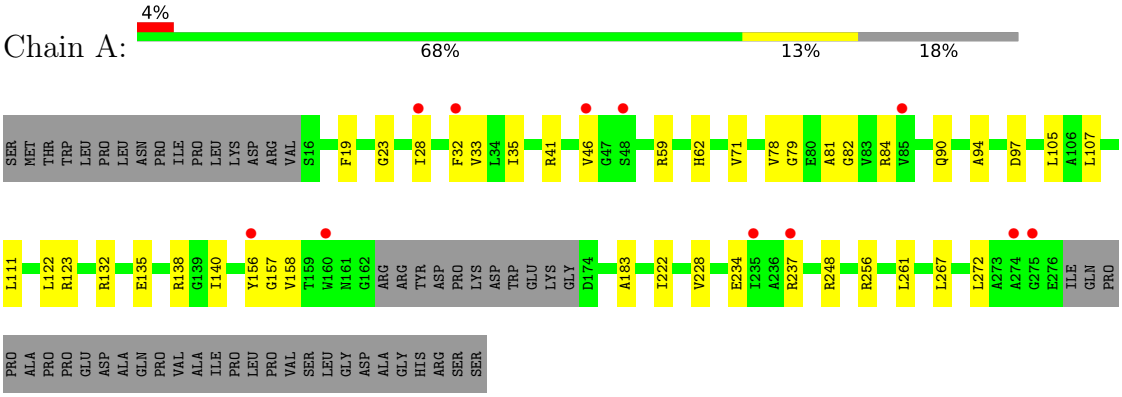
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		
5	D	1	Total	Mg	0	0
			1	1		
5	G	1	Total	Mg	0	0
			1	1		
5	H	1	Total	Mg	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

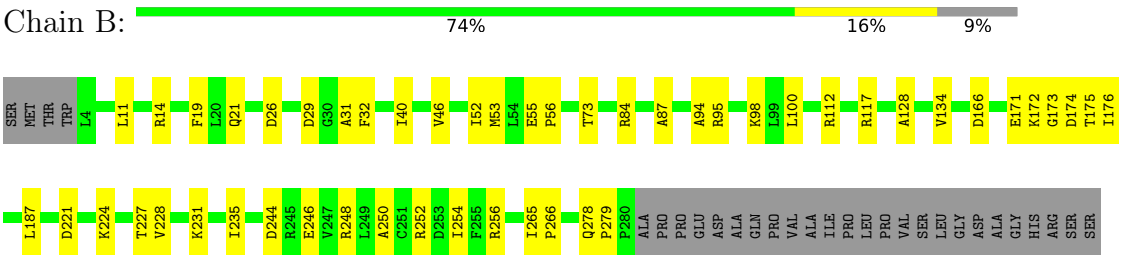
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain A:



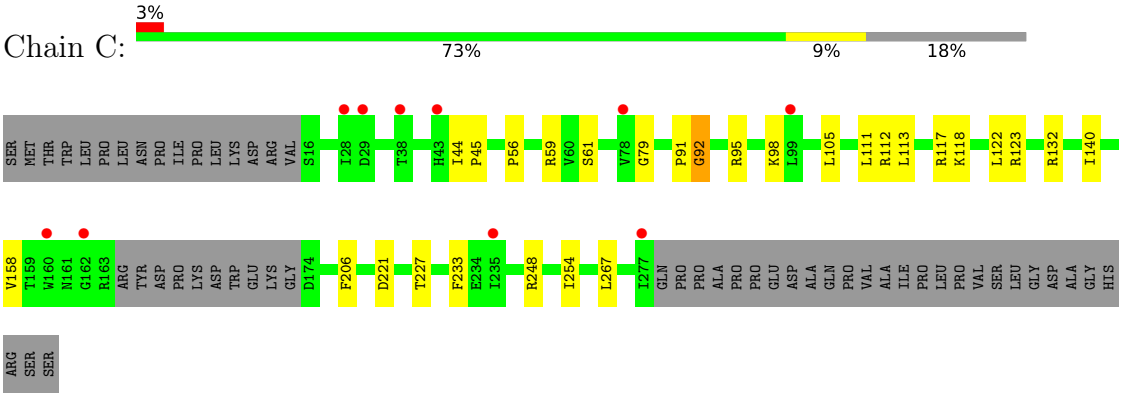
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain B:



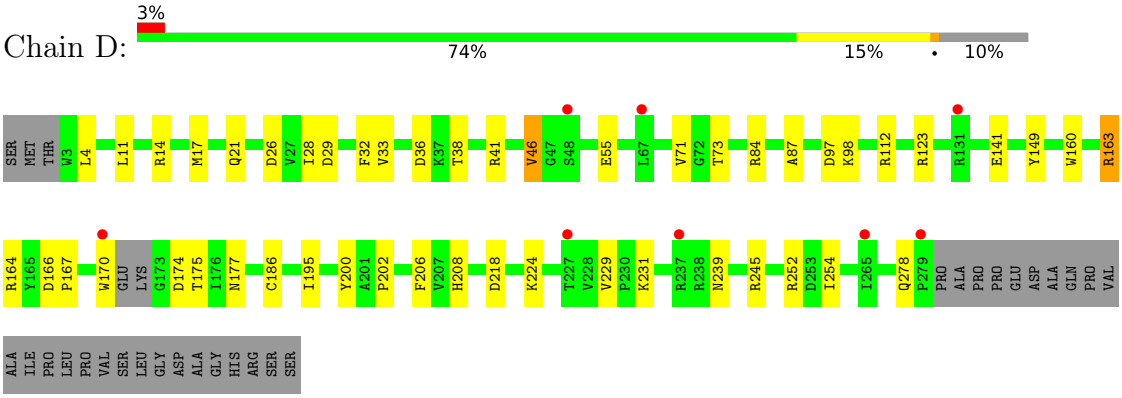
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain C:



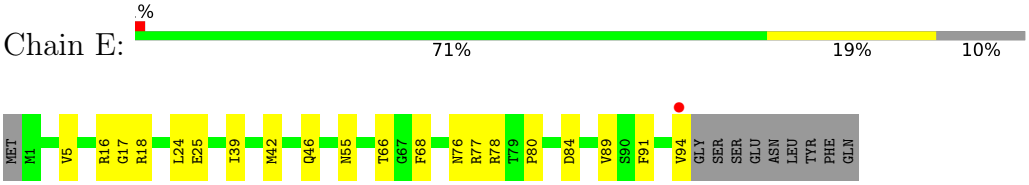
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain D:



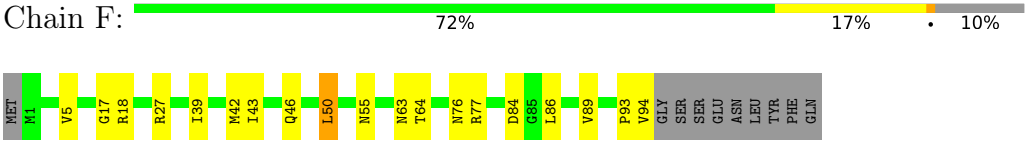
• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain E:



• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain F:

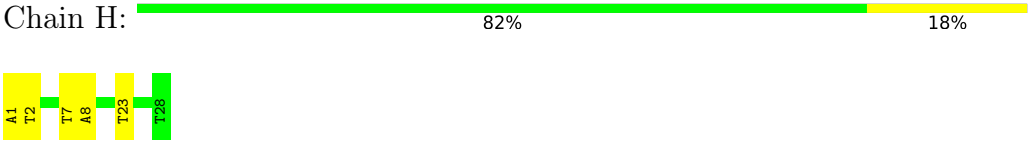


• Molecule 3: DNA (28-MER)

Chain G:

• Molecule 4: DNA (28-MER)

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.66Å 165.93Å 167.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.48 – 2.95 46.48 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.48-2.95) 98.1 (46.48-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.256 0.233 , 0.256	Depositor DCC
R_{free} test set	2641 reflections (5.87%)	wwPDB-VP
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 20.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.109 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10719	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: MG

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	0.22	0/1940	0.43	0/2628
1	B	0.22	0/2179	0.43	0/2957
1	C	0.22	0/1959	0.43	0/2653
1	D	0.21	0/2168	0.44	0/2942
2	E	0.21	0/753	0.42	0/1024
2	F	0.20	0/753	0.39	0/1024
3	G	0.46	0/652	0.79	0/1005
4	H	0.52	0/627	1.04	0/966
All	All	0.26	0/11031	0.52	0/15199

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	1907	0	1963	27	0
1	B	2136	0	2202	35	0
1	C	1926	0	1987	17	0
1	D	2125	0	2185	34	0
2	E	739	0	756	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	739	0	756	21	0
3	G	578	0	314	10	0
4	H	564	0	324	4	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	10719	0	10487	136	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 7.

All (136) 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)
2:E:5:VAL:HG21	2:F:5:VAL:HG21	1.54	0.86
1:A:59:ARG:NH2	1:B:26:ASP:OD1	2.13	0.81
1:C:59:ARG:NH2	1:D:26:ASP:OD1	2.14	0.81
1:A:28:ILE:HD13	1:A:41:ARG:HE	1.51	0.75
2:E:55:ASN:HD22	2:F:27:ARG:HH21	1.33	0.73
1:D:123:ARG:NH1	1:D:141:GLU:OE1	2.22	0.73
1:A:234:GLU:HG3	1:A:237:ARG:HH21	1.56	0.69
1:A:59:ARG:NH1	4:H:2:DT:OP1	2.26	0.68
1:A:78:VAL:HB	1:A:82:GLY:HA2	1.77	0.67
1:B:252:ARG:NH2	2:F:84:ASP:O	2.29	0.66
1:A:84:ARG:NH1	3:G:25:DG:OP1	2.30	0.64
1:A:28:ILE:HD11	1:A:35:ILE:HD11	1.79	0.64
1:A:28:ILE:HG13	1:A:33:VAL:HG21	1.80	0.64
1:B:244:ASP:O	1:B:248:ARG:HG2	1.97	0.63
2:E:66:THR:OG1	2:E:68:PHE:O	2.17	0.63
1:B:256:ARG:HD2	2:F:64:THR:HA	1.81	0.62
1:B:174:ASP:O	1:B:176:ILE:N	2.31	0.62
1:C:158:VAL:HG21	1:C:233:PHE:HD2	1.65	0.61
2:E:76:ASN:HD22	2:E:78:ARG:H	1.47	0.61
1:C:112:ARG:HG3	1:C:206:PHE:HD2	1.68	0.59
1:B:171:GLU:O	1:B:173:GLY:N	2.34	0.59
1:D:17:MET:O	1:D:252:ARG:NH1	2.34	0.59
1:A:105:LEU:HD23	1:A:111:LEU:HD23	1.84	0.58
1:A:123:ARG:HD3	1:A:222:ILE:HA	1.85	0.58
2:E:18:ARG:NH1	2:E:46:GLN:OE1	2.37	0.58
1:A:156:TYR:O	1:A:158:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:NH1	2:F:86:LEU:HB2	2.19	0.57
1:C:248:ARG:NH1	4:H:23:DT:OP1	2.36	0.57
1:C:105:LEU:HD23	1:C:111:LEU:HD23	1.88	0.56
2:E:16:ARG:NH2	2:E:25:GLU:OE2	2.36	0.55
1:D:11:LEU:HD12	1:D:14:ARG:HD2	1.89	0.55
1:A:90:GLN:HB3	1:A:94:ALA:HB2	1.88	0.55
4:H:7:DT:H2"	4:H:8:DA:C8	2.42	0.54
1:D:4:LEU:HG	2:F:50:LEU:HD11	1.89	0.54
1:B:252:ARG:HH12	2:F:86:LEU:HB2	1.73	0.54
1:B:227:THR:HB	1:B:254:ILE:HG21	1.90	0.54
2:E:77:ARG:HH12	2:E:94:VAL:HG13	1.72	0.54
2:F:18:ARG:NH1	2:F:46:GLN:OE1	2.42	0.53
2:E:76:ASN:ND2	2:E:78:ARG:H	2.06	0.52
1:D:41:ARG:HB2	2:E:91:PHE:HB3	1.92	0.52
1:B:231:LYS:HG3	1:B:250:ALA:HB1	1.91	0.52
3:G:20:DA:H2'	3:G:21:DA:C8	2.43	0.52
1:A:97:ASP:N	1:A:97:ASP:OD1	2.42	0.52
1:B:46:VAL:HG12	1:B:52:ILE:HD11	1.92	0.52
1:A:135:GLU:OE1	1:A:138:ARG:NH1	2.43	0.51
1:D:29:ASP:O	2:F:17:GLY:HA3	2.10	0.51
1:B:166:ASP:OD1	1:B:166:ASP:N	2.41	0.51
2:F:39:ILE:O	2:F:43:ILE:HG12	2.11	0.51
1:B:235:ILE:HD12	1:B:246:GLU:HB3	1.93	0.51
1:D:36:ASP:OD2	1:D:38:THR:OG1	2.27	0.51
2:F:77:ARG:HH22	2:F:94:VAL:HG13	1.75	0.51
1:C:123:ARG:NH2	1:C:221:ASP:HB3	2.26	0.51
1:C:158:VAL:HG21	1:C:233:PHE:CD2	2.46	0.50
1:D:195:ILE:HG23	1:D:200:TYR:HB2	1.94	0.50
3:G:7:DC:H2"	3:G:8:DA:C8	2.46	0.50
1:B:95:ARG:HD2	1:B:98:LYS:HD2	1.93	0.50
2:E:39:ILE:O	2:E:42:MET:HG3	2.10	0.50
1:B:84:ARG:HH21	1:B:87:ALA:HB3	1.76	0.50
1:B:256:ARG:NH1	2:F:63:ASN:O	2.45	0.49
1:C:59:ARG:NH1	3:G:2:DA:OP1	2.45	0.49
1:B:19:PHE:CE1	1:B:248:ARG:HD2	2.48	0.49
1:D:167:PRO:HA	1:D:170:TRP:CE2	2.48	0.49
1:C:132:ARG:NH1	1:C:140:ILE:HD11	2.28	0.49
1:D:4:LEU:HB3	2:F:18:ARG:HH22	1.78	0.48
1:A:79:GLY:N	1:A:84:ARG:O	2.45	0.48
1:A:248:ARG:NH1	3:G:23:DT:OP1	2.40	0.48
1:A:19:PHE:HZ	1:A:261:LEU:HD23	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:ARG:NH2	1:D:206:PHE:O	2.46	0.48
1:D:149:TYR:CE2	1:D:163:ARG:HG3	2.48	0.48
2:F:55:ASN:OD1	2:F:76:ASN:ND2	2.42	0.47
1:D:4:LEU:HB3	2:F:18:ARG:NH2	2.30	0.47
1:B:221:ASP:HA	1:B:224:LYS:HG2	1.97	0.46
1:D:46:VAL:O	1:D:73:THR:OG1	2.29	0.46
3:G:25:DG:H4'	3:G:26:DG:H5"	1.97	0.46
1:B:29:ASP:O	2:E:17:GLY:HA3	2.15	0.46
1:C:95:ARG:HD2	1:C:98:LYS:HD2	1.97	0.46
1:B:19:PHE:CZ	1:B:53:MET:HG3	2.50	0.46
1:C:118:LYS:HE3	1:C:122:LEU:HD11	1.98	0.46
2:E:55:ASN:HD22	2:F:27:ARG:NH2	2.07	0.46
1:C:227:THR:HG22	1:C:254:ILE:HD13	1.97	0.46
1:D:160:TRP:HH2	1:D:163:ARG:HG2	1.79	0.46
1:A:19:PHE:CZ	1:A:261:LEU:HD23	2.51	0.46
1:C:56:PRO:HD3	1:C:79:GLY:HA2	1.98	0.45
1:A:81:ALA:HB2	1:A:256:ARG:HE	1.82	0.45
1:D:164:ARG:HH22	1:D:174:ASP:HB3	1.81	0.45
1:D:224:LYS:HG2	1:D:229:VAL:HG23	1.98	0.45
1:B:21:GLN:HB3	1:B:55:GLU:HB2	1.99	0.45
1:D:21:GLN:HB3	1:D:55:GLU:HB2	1.99	0.45
1:D:112:ARG:HG3	1:D:206:PHE:HD2	1.81	0.45
1:D:164:ARG:HH21	1:D:177:ASN:HD22	1.64	0.45
1:B:11:LEU:HD12	1:B:14:ARG:HD2	1.98	0.45
2:F:42:MET:O	2:F:46:GLN:HG2	2.17	0.44
1:A:62:HIS:CG	1:B:56:PRO:HA	2.52	0.44
1:D:164:ARG:HE	1:D:177:ASN:ND2	2.15	0.44
3:G:9:DG:H2"	3:G:10:DA:C8	2.52	0.44
1:B:46:VAL:O	1:B:73:THR:OG1	2.34	0.44
1:B:40:ILE:HG22	2:F:93:PRO:HD3	2.00	0.44
1:A:23:GLY:HA2	4:H:1:DA:H4'	2.00	0.44
1:A:132:ARG:NH2	1:A:140:ILE:HD11	2.33	0.44
1:D:245:ARG:HG3	2:E:84:ASP:HA	1.99	0.44
1:C:92:GLY:HA3	1:D:202:PRO:HD2	2.00	0.44
2:E:55:ASN:ND2	2:E:76:ASN:OD1	2.50	0.44
1:B:117:ARG:NH2	1:B:128:ALA:O	2.51	0.43
2:F:46:GLN:O	2:F:50:LEU:HB2	2.19	0.43
1:A:84:ARG:HD3	1:A:84:ARG:HA	1.80	0.43
1:B:19:PHE:CZ	1:B:248:ARG:HD2	2.53	0.43
1:D:28:ILE:HG13	1:D:33:VAL:HG21	1.99	0.43
1:B:278:GLN:H	1:B:278:GLN:CD	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:HIS:ND1	1:D:218:ASP:OD1	2.38	0.43
1:D:231:LYS:HB2	1:D:254:ILE:HD11	2.01	0.43
2:E:80:PRO:HA	2:E:89:VAL:HA	2.00	0.43
1:C:122:LEU:HD13	1:C:267:LEU:HD11	2.00	0.42
1:B:227:THR:HB	1:B:254:ILE:CG2	2.49	0.42
1:D:17:MET:HE1	1:D:186:CYS:HB3	2.00	0.42
1:A:107:LEU:HD21	1:B:100:LEU:HB3	2.01	0.42
1:D:97:ASP:OD1	1:D:98:LYS:N	2.53	0.42
1:B:31:ALA:HB2	2:E:17:GLY:O	2.20	0.41
3:G:12:DC:H2"	3:G:13:DG:C8	2.54	0.41
3:G:26:DG:H8	3:G:27:DG:C8	2.38	0.41
1:B:187:LEU:HD22	1:B:228:VAL:HG21	2.03	0.41
1:A:46:VAL:HB	1:A:71:VAL:HG21	2.02	0.41
1:C:44:ILE:HA	1:C:45:PRO:HD3	1.89	0.41
2:E:24:LEU:HD11	2:F:89:VAL:HG12	2.03	0.41
1:A:183:ALA:HB1	1:A:228:VAL:HG12	2.03	0.41
1:D:84:ARG:HH21	1:D:87:ALA:HB3	1.86	0.41
2:F:77:ARG:HH12	2:F:94:VAL:HG13	1.84	0.41
1:A:122:LEU:HD13	1:A:267:LEU:HD11	2.03	0.41
1:C:113:LEU:O	1:C:117:ARG:HG3	2.20	0.41
1:D:166:ASP:HA	1:D:167:PRO:HD3	1.90	0.41
1:D:175:THR:HG21	1:D:239:ASN:HA	2.02	0.41
1:B:278:GLN:HA	1:B:279:PRO:HD3	1.92	0.41
1:D:278:GLN:H	1:D:278:GLN:CD	2.24	0.41
1:B:112:ARG:NH1	1:B:134:VAL:HG21	2.36	0.40
1:D:46:VAL:HB	1:D:71:VAL:HG21	2.03	0.40
1:B:265:ILE:HB	1:B:266:PRO:HD3	2.03	0.40
3:G:13:DG:H2"	3:G:14:DA:C8	2.56	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	246/306 (80%)	236 (96%)	9 (4%)	1 (0%)	34 69
1	B	275/306 (90%)	261 (95%)	11 (4%)	3 (1%)	14 46
1	C	248/306 (81%)	235 (95%)	11 (4%)	2 (1%)	19 53
1	D	271/306 (89%)	262 (97%)	9 (3%)	0	100 100
2	E	92/104 (88%)	87 (95%)	5 (5%)	0	100 100
2	F	92/104 (88%)	87 (95%)	5 (5%)	0	100 100
All	All	1224/1432 (86%)	1168 (95%)	50 (4%)	6 (0%)	29 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	175	THR
1	C	91	PRO
1	A	157	GLY
1	B	94	ALA
1	C	92	GLY
1	B	172	LYS

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	197/246 (80%)	195 (99%)	2 (1%)	76 90
1	B	223/246 (91%)	222 (100%)	1 (0%)	91 96
1	C	199/246 (81%)	198 (100%)	1 (0%)	88 95
1	D	221/246 (90%)	218 (99%)	3 (1%)	67 86
2	E	79/88 (90%)	79 (100%)	0	100 100
2	F	79/88 (90%)	78 (99%)	1 (1%)	69 87
All	All	998/1160 (86%)	990 (99%)	8 (1%)	81 92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	PHE
1	A	272	LEU
1	B	32	PHE
1	C	61	SER
1	D	32	PHE
1	D	46	VAL
1	D	163	ARG
2	F	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	55	ASN
2	E	76	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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	250/306 (81%)	0.61	11 (4%) 34 21	42, 70, 97, 113	0
1	B	277/306 (90%)	0.43	0 100 100	38, 60, 91, 108	0
1	C	252/306 (82%)	0.61	10 (3%) 38 25	47, 70, 103, 115	0
1	D	275/306 (89%)	0.53	8 (2%) 51 35	43, 63, 88, 121	0
2	E	94/104 (90%)	0.39	1 (1%) 80 65	41, 54, 74, 93	0
2	F	94/104 (90%)	0.50	0 100 100	39, 53, 76, 85	0
3	G	28/28 (100%)	0.01	0 100 100	49, 61, 116, 126	0
4	H	28/28 (100%)	-0.07	0 100 100	46, 61, 101, 111	0
All	All	1298/1488 (87%)	0.50	30 (2%) 60 43	38, 63, 96, 126	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	SER	4.7
1	A	28	ILE	3.8
1	A	46	VAL	3.8
1	D	48	SER	3.7
1	C	28	ILE	3.4
1	A	275	GLY	3.3
1	A	237	ARG	3.0
1	A	32	PHE	3.0
1	C	43	HIS	2.9
1	C	160	TRP	2.8
1	C	235	ILE	2.8
2	E	94	VAL	2.6
1	D	265	ILE	2.6
1	D	170	TRP	2.5
1	A	235	ILE	2.5
1	D	279	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	237	ARG	2.5
1	A	160	TRP	2.5
1	C	99	LEU	2.4
1	C	162	GLY	2.3
1	D	227	THR	2.3
1	A	156	TYR	2.2
1	C	277	ILE	2.2
1	C	38	THR	2.2
1	D	131	ARG	2.1
1	C	29	ASP	2.1
1	A	85	VAL	2.1
1	A	274	ALA	2.1
1	C	78	VAL	2.1
1	D	67	LEU	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	MG	H	101	1/1	0.88	0.29	63,63,63,63	0
5	MG	G	101	1/1	0.90	0.40	44,44,44,44	0
5	MG	B	401	1/1	0.90	0.27	44,44,44,44	0
5	MG	B	402	1/1	0.92	0.16	30,30,30,30	0
5	MG	D	401	1/1	0.96	0.15	53,53,53,53	0

6.5 Other polymers (i)

There are no such residues in this entry.