Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:32 PM GMT

PDB ID	:	4P6I
Title	:	Crystal structure of the Cas1-Cas2 complex from Escherichia coli
Authors	:	Nunez, J.K.; Kranzusch, P.J.; Noeske, J.; Doudna, J.A.
Deposited on	:	2014-03-25
Resolution	:	2.30 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.

The following versions of software and data (see references (1)) were used in the production of this report:

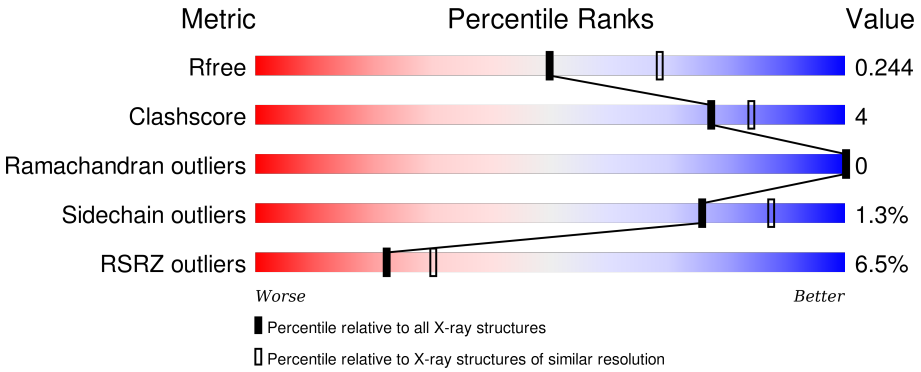
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	103	6% 81% 17%
1	B	103	4% 82% 13% 6%
2	C	305	8% 80% 8% 11%
2	D	305	5% 87% 8% 6%
2	E	305	8% 78% 7% 15%

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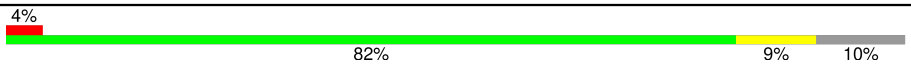
Mol	Chain	Length	Quality of chain
2	F	305	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10450 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 endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			792	507	136	145	4			
1	B	97	Total	C	N	O	S	0	0	0
			755	483	131	137	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	-	expression tag	UNP P45956
A	96	SER	-	expression tag	UNP P45956
A	97	SER	-	expression tag	UNP P45956
A	98	GLU	-	expression tag	UNP P45956
A	99	ASN	-	expression tag	UNP P45956
A	100	LEU	-	expression tag	UNP P45956
A	101	TYR	-	expression tag	UNP P45956
A	102	PHE	-	expression tag	UNP P45956
A	103	GLN	-	expression tag	UNP P45956
B	95	GLY	-	expression tag	UNP P45956
B	96	SER	-	expression tag	UNP P45956
B	97	SER	-	expression tag	UNP P45956
B	98	GLU	-	expression tag	UNP P45956
B	99	ASN	-	expression tag	UNP P45956
B	100	LEU	-	expression tag	UNP P45956
B	101	TYR	-	expression tag	UNP P45956
B	102	PHE	-	expression tag	UNP P45956
B	103	GLN	-	expression tag	UNP P45956

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	270	Total	C	N	O	S	0	0	0
			2080	1327	371	375	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	288	Total	C	N	O	S	0	0	0
			2200	1409	388	396	7			
2	E	259	Total	C	N	O	S	0	0	0
			1979	1262	353	357	7			
2	F	276	Total	C	N	O	S	0	0	0
			2119	1356	376	380	7			

- Molecule 3 is water.

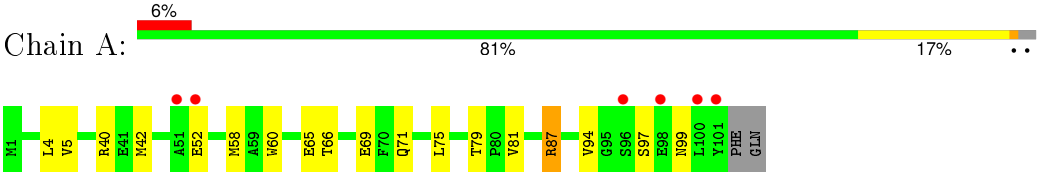
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		
3	B	55	Total	O	0	0
			55	55		
3	C	86	Total	O	0	0
			86	86		
3	D	136	Total	O	0	0
			136	136		
3	E	66	Total	O	0	0
			66	66		
3	F	116	Total	O	0	0
			116	116		

3 Residue-property plots (i)

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.

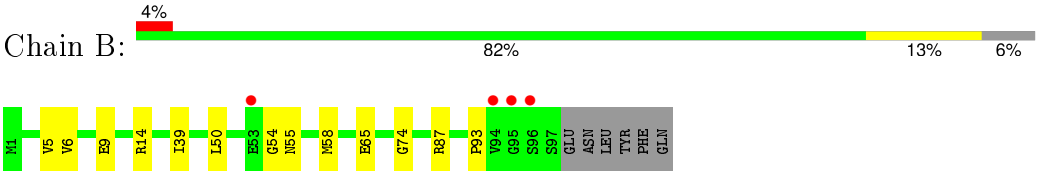
- Molecule 1: CRISPR-associated endoribonuclease Cas2

Chain A:



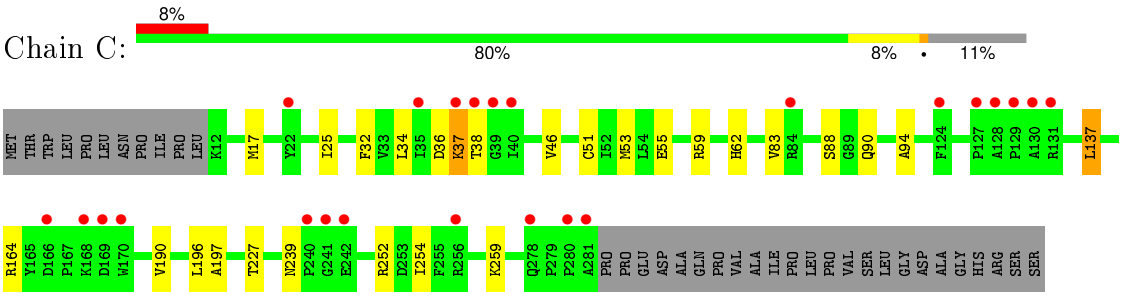
- Molecule 1: CRISPR-associated endoribonuclease Cas2

Chain B:



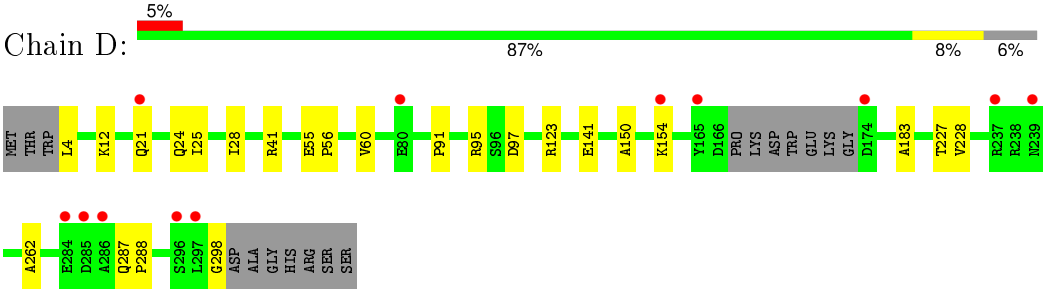
- Molecule 2: CRISPR-associated endonuclease Cas1

Chain C:



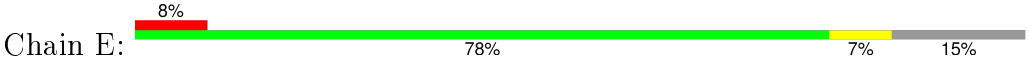
- Molecule 2: CRISPR-associated endonuclease Cas1

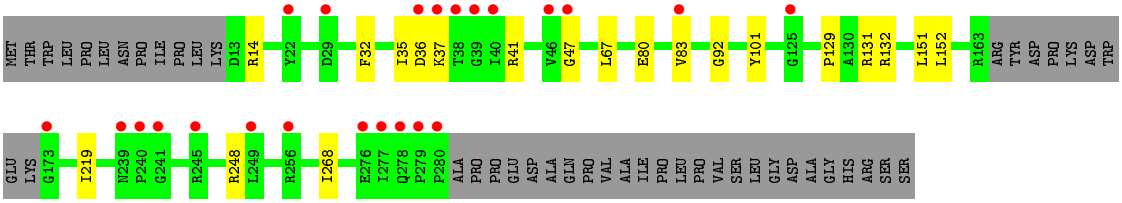
Chain D:



- Molecule 2: CRISPR-associated endonuclease Cas1

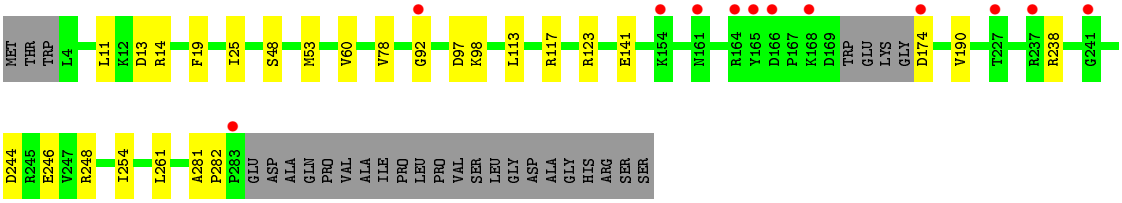
Chain E:





- Molecule 2: CRISPR-associated endonuclease Cas1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.88Å 125.70Å 99.31Å 90.00° 102.74° 90.00°	Depositor
Resolution (Å)	62.85 – 2.30 62.85 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (62.85-2.30) 97.2 (62.85-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.225 , 0.245 0.222 , 0.244	Depositor DCC
R_{free} test set	2014 reflections (2.06%)	DCC
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.0	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 97929 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10450	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	0/807	0.40	0/1097
1	B	0.21	0/769	0.37	0/1045
2	C	0.21	0/2120	0.37	0/2873
2	D	0.22	0/2244	0.38	0/3051
2	E	0.21	0/2014	0.38	0/2729
2	F	0.21	0/2161	0.38	0/2934
All	All	0.21	0/10115	0.38	0/13729

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	792	0	801	13	0
1	B	755	0	769	9	0
2	C	2080	0	2136	14	0
2	D	2200	0	2272	18	0
2	E	1979	0	2038	12	0
2	F	2119	0	2188	17	0
3	A	66	0	0	5	0
3	B	55	0	0	1	0
3	C	86	0	0	0	0
3	D	136	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	66	0	0	2	0
3	F	116	0	0	2	0
All	All	10450	0	10204	74	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 4.

All (74) 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:F:113:LEU:O	3:F:501:HOH:O	2.00	0.79
2:F:238:ARG:NH1	2:F:246:GLU:OE2	2.17	0.77
1:B:65:GLU:OE2	3:B:242:HOH:O	2.04	0.75
2:F:11:LEU:HA	2:F:14:ARG:HD3	1.79	0.65
2:D:227:THR:OG1	3:D:422:HOH:O	2.13	0.65
2:D:123:ARG:NH1	2:D:141:GLU:OE2	2.31	0.63
2:E:14:ARG:NH1	2:E:47:GLY:O	2.31	0.62
1:A:94:VAL:HG23	1:A:97:SER:HB2	1.82	0.62
1:B:39:ILE:HD11	2:F:13:ASP:HB3	1.84	0.60
2:D:4:LEU:N	3:D:522:HOH:O	2.35	0.59
2:D:21:GLN:HA	2:D:55:GLU:HB2	1.87	0.56
2:F:244:ASP:O	2:F:248:ARG:HG2	2.07	0.53
1:A:99:ASN:ND2	3:A:263:HOH:O	2.41	0.52
2:F:190:VAL:HB	2:F:261:LEU:HD21	1.92	0.52
2:E:101:TYR:OH	3:E:461:HOH:O	2.19	0.51
1:A:81:VAL:HB	2:D:298:GLY:HA3	1.92	0.51
2:E:36:ASP:OD1	2:E:37:LYS:N	2.33	0.51
2:F:117:ARG:N	3:F:501:HOH:O	2.09	0.51
2:E:131:ARG:NH2	2:E:132:ARG:HH12	2.10	0.50
2:E:35:ILE:HG13	2:E:41:ARG:HG2	1.93	0.50
1:B:87:ARG:HH11	1:B:87:ARG:HA	1.78	0.49
2:C:17:MET:HG2	2:C:51:CYS:HB3	1.94	0.49
2:F:19:PHE:CZ	2:F:248:ARG:HD2	2.47	0.48
2:C:59:ARG:HE	2:D:24:GLN:HE22	1.60	0.48
2:C:37:LYS:HD2	2:C:38:THR:N	2.28	0.48
2:E:219:ILE:HG12	2:E:268:ILE:HG12	1.95	0.48
2:F:174:ASP:N	2:F:174:ASP:OD1	2.47	0.48
1:A:69:GLU:OE2	1:A:87:ARG:NH1	2.47	0.47
2:F:97:ASP:OD1	2:F:98:LYS:N	2.47	0.47
2:E:92:GLY:HA2	2:F:92:GLY:HA2	1.97	0.47
2:E:80:GLU:OE1	2:E:248:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NH2	3:A:225:HOH:O	2.48	0.46
2:E:36:ASP:OD1	2:E:37:LYS:HG3	2.15	0.46
2:C:227:THR:HG22	2:C:254:ILE:HD13	1.98	0.46
2:C:25:ILE:HG12	2:C:34:LEU:HD23	1.97	0.46
2:F:14:ARG:HG2	2:F:48:SER:HA	1.98	0.46
2:C:55:GLU:OE1	2:C:252:ARG:NH2	2.44	0.46
2:C:32:PHE:CG	2:C:46:VAL:HG21	2.51	0.46
2:C:62:HIS:CG	2:D:56:PRO:HA	2.51	0.46
2:D:150:ALA:O	2:D:154:LYS:HD3	2.16	0.46
2:F:25:ILE:HG12	2:F:60:VAL:HG12	1.98	0.45
2:F:123:ARG:NH1	2:F:141:GLU:OE2	2.48	0.45
2:E:83:VAL:O	3:E:409:HOH:O	2.21	0.45
2:C:196:LEU:HD11	2:D:91:PRO:HB3	1.98	0.45
1:B:6:VAL:HG22	1:B:58:MET:HG3	1.99	0.45
2:E:129:PRO:HG2	2:E:132:ARG:HG2	1.99	0.44
2:C:53:MET:HE1	2:C:190:VAL:HA	1.99	0.44
2:F:281:ALA:HA	2:F:282:PRO:HD3	1.89	0.44
1:A:66:THR:HG21	1:A:87:ARG:HB3	2.00	0.44
2:C:88:SER:HB3	2:D:91:PRO:HA	1.99	0.44
2:D:183:ALA:HB1	2:D:228:VAL:HG13	1.99	0.44
2:C:90:GLN:HB3	2:C:94:ALA:HB2	2.00	0.43
2:D:25:ILE:HD11	2:D:60:VAL:HG13	2.01	0.43
1:A:40:ARG:HD3	1:A:60:TRP:CD2	2.54	0.42
1:B:54:GLY:O	1:B:74:GLY:HA3	2.19	0.42
1:A:52:GLU:OE1	1:A:52:GLU:N	2.51	0.42
1:B:14:ARG:HD3	1:B:50:LEU:HD22	2.01	0.42
1:B:9:GLU:HB3	1:B:55:ASN:HB3	2.01	0.42
1:A:65:GLU:OE1	3:A:229:HOH:O	2.21	0.42
2:D:28:ILE:HG21	2:D:41:ARG:NH1	2.35	0.41
2:C:137:LEU:HD12	2:C:137:LEU:HA	1.93	0.41
1:A:79:THR:HG23	3:A:211:HOH:O	2.20	0.41
2:D:287:GLN:NE2	3:D:451:HOH:O	2.52	0.41
2:F:254:ILE:HA	2:F:254:ILE:HD13	1.91	0.41
1:A:71:GLN:NE2	3:A:227:HOH:O	2.45	0.41
2:C:51:CYS:HB2	2:C:197:ALA:HB2	2.02	0.41
1:B:93:PRO:HB3	2:D:41:ARG:CZ	2.50	0.41
2:D:12:LYS:HG3	2:D:262:ALA:HB2	2.03	0.41
2:F:19:PHE:CZ	2:F:53:MET:HG3	2.56	0.40
1:A:4:LEU:HD11	1:A:58:MET:HG3	2.03	0.40
2:D:95:ARG:HB3	2:D:97:ASP:OD1	2.21	0.40
1:A:5:VAL:HG11	1:B:5:VAL:HG11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:32:PHE:HD2	2:E:67:LEU:HD23	1.87	0.40
2:D:287:GLN:HA	2:D:288:PRO:HD3	1.97	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	99/103 (96%)	96 (97%)	3 (3%)	0	100	100
1	B	95/103 (92%)	92 (97%)	3 (3%)	0	100	100
2	C	268/305 (88%)	262 (98%)	6 (2%)	0	100	100
2	D	284/305 (93%)	278 (98%)	6 (2%)	0	100	100
2	E	255/305 (84%)	248 (97%)	7 (3%)	0	100	100
2	F	272/305 (89%)	268 (98%)	4 (2%)	0	100	100
All	All	1273/1426 (89%)	1244 (98%)	29 (2%)	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	85/87 (98%)	82 (96%)	3 (4%)	43	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	81/87 (93%)	81 (100%)	0	100 100
2	C	215/245 (88%)	208 (97%)	7 (3%)	45 61
2	D	231/245 (94%)	231 (100%)	0	100 100
2	E	205/245 (84%)	203 (99%)	2 (1%)	82 91
2	F	222/245 (91%)	221 (100%)	1 (0%)	92 97
All	All	1039/1154 (90%)	1026 (99%)	13 (1%)	76 87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	MET
1	A	75	LEU
1	A	87	ARG
2	C	36	ASP
2	C	37	LYS
2	C	83	VAL
2	C	137	LEU
2	C	164	ARG
2	C	239	ASN
2	C	259	LYS
2	E	151	LEU
2	E	152	LEU
2	F	78	VAL

Some 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 carbohydrates 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	101/103 (98%)	0.62	6 (5%)	26	34	34, 48, 76, 93	0
1	B	97/103 (94%)	0.50	4 (4%)	41	50	36, 46, 68, 89	0
2	C	270/305 (88%)	0.60	24 (8%)	12	17	39, 54, 87, 110	0
2	D	288/305 (94%)	0.44	15 (5%)	31	39	36, 49, 80, 95	0
2	E	259/305 (84%)	0.49	23 (8%)	12	17	38, 55, 84, 94	0
2	F	276/305 (90%)	0.43	12 (4%)	39	48	36, 52, 86, 101	0
All	All	1291/1426 (90%)	0.50	84 (6%)	22	30	34, 51, 84, 110	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	129	PRO	16.2
1	B	95	GLY	9.2
2	C	22	TYR	6.8
2	C	130	ALA	6.7
2	E	280	PRO	4.9
2	C	38	THR	4.8
1	B	94	VAL	4.6
2	F	283	PRO	4.5
1	A	96	SER	4.3
1	B	96	SER	4.2
2	C	281	ALA	4.1
2	D	80	GLU	4.0
1	A	101	TYR	4.0
2	E	279	PRO	3.9
2	C	168	LYS	3.9
2	F	92	GLY	3.8
2	F	237	ARG	3.7
2	F	165	TYR	3.7
1	A	51	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	173	GLY	3.6
2	D	165	TYR	3.5
2	C	256	ARG	3.4
2	E	38	THR	3.3
2	E	40	ILE	3.2
2	E	29	ASP	3.1
2	C	131	ARG	3.1
2	C	37	LYS	3.0
2	F	161	ASN	3.0
2	C	280	PRO	3.0
2	E	249	LEU	3.0
2	E	278	GLN	2.9
2	C	240	PRO	2.9
2	D	237	ARG	2.8
2	E	125	GLY	2.8
2	D	174	ASP	2.8
2	C	39	GLY	2.8
2	F	174	ASP	2.8
1	A	52	GLU	2.7
2	C	35	ILE	2.7
2	C	170	TRP	2.7
2	F	241	GLY	2.7
2	E	276	GLU	2.7
2	C	40	ILE	2.6
2	E	241	GLY	2.6
2	C	242	GLU	2.6
2	D	21	GLN	2.6
2	F	164	ARG	2.6
2	C	241	GLY	2.5
2	D	297	LEU	2.5
2	E	277	ILE	2.5
2	E	36	ASP	2.5
2	D	241	GLY	2.4
2	E	37	LYS	2.4
2	C	127	PRO	2.4
2	E	39	GLY	2.3
2	E	22	TYR	2.3
2	E	240	PRO	2.3
2	F	227	THR	2.3
2	F	166	ASP	2.3
2	D	284	GLU	2.3
2	F	168	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	84	ARG	2.3
2	D	285	ASP	2.2
2	D	154	LYS	2.2
2	C	128	ALA	2.2
2	D	245	ARG	2.2
2	D	239	ASN	2.2
1	B	53	GLU	2.2
2	E	245	ARG	2.2
2	D	296	SER	2.2
2	D	240	PRO	2.1
1	A	100	LEU	2.1
2	C	169	ASP	2.1
2	C	278	GLN	2.1
2	E	46	VAL	2.1
2	D	286	ALA	2.1
2	E	256	ARG	2.1
2	F	154	LYS	2.1
2	C	124	PHE	2.1
1	A	98	GLU	2.1
2	E	83	VAL	2.1
2	C	166	ASP	2.0
2	E	47	GLY	2.0
2	E	239	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.