Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 08:10 AM EDT

PDB ID	:	4QDL
Title	:	Crystal structure of E.coli Cas1-Cas2 complex
Authors	:	Tamulaitiene, G.; Sinkunas, T.; Silanskas, A.; Gasiunas, G.; Grazulis, S.; Siksnys, V.
Deposited on	:	2014-05-14
Resolution	:	2.70 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:

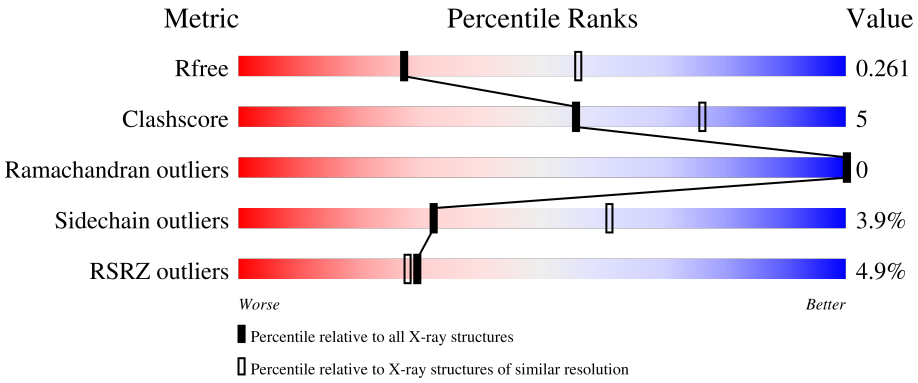
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	305	4% 74% 10% 15%
1	B	305	78% 10% • 11%
1	C	305	12% 62% 15% • 22%
1	D	305	3% 76% 13% 11%
2	E	104	73% 14% • 11%

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Mol	Chain	Length	Quality of chain
2	F	104	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9133 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	258	Total	C	N	O	S	0	0	0
			1817	1176	308	326	7			
1	B	272	Total	C	N	O	S	0	1	0
			2071	1330	368	366	7			
1	C	239	Total	C	N	O	S	0	0	0
			1702	1107	285	303	7			
1	D	271	Total	C	N	O	S	0	0	0
			2030	1307	356	360	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	93	Total	C	N	O	S	0	0	0
			731	470	127	131	3			
2	F	94	Total	C	N	O	S	0	0	0
			726	469	124	130	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	95	LEU	-	expression tag	UNP P45956
E	96	GLU	-	expression tag	UNP P45956
E	97	SER	-	expression tag	UNP P45956
E	98	GLY	-	expression tag	UNP P45956
E	99	HIS	-	expression tag	UNP P45956
E	100	HIS	-	expression tag	UNP P45956
E	101	HIS	-	expression tag	UNP P45956
E	102	HIS	-	expression tag	UNP P45956
E	103	HIS	-	expression tag	UNP P45956
E	104	HIS	-	expression tag	UNP P45956
F	95	LEU	-	expression tag	UNP P45956
F	96	GLU	-	expression tag	UNP P45956

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Chain	Residue	Modelled	Actual	Comment	Reference
F	97	SER	-	expression tag	UNP P45956
F	98	GLY	-	expression tag	UNP P45956
F	99	HIS	-	expression tag	UNP P45956
F	100	HIS	-	expression tag	UNP P45956
F	101	HIS	-	expression tag	UNP P45956
F	102	HIS	-	expression tag	UNP P45956
F	103	HIS	-	expression tag	UNP P45956
F	104	HIS	-	expression tag	UNP P45956

- Molecule 3 is water.

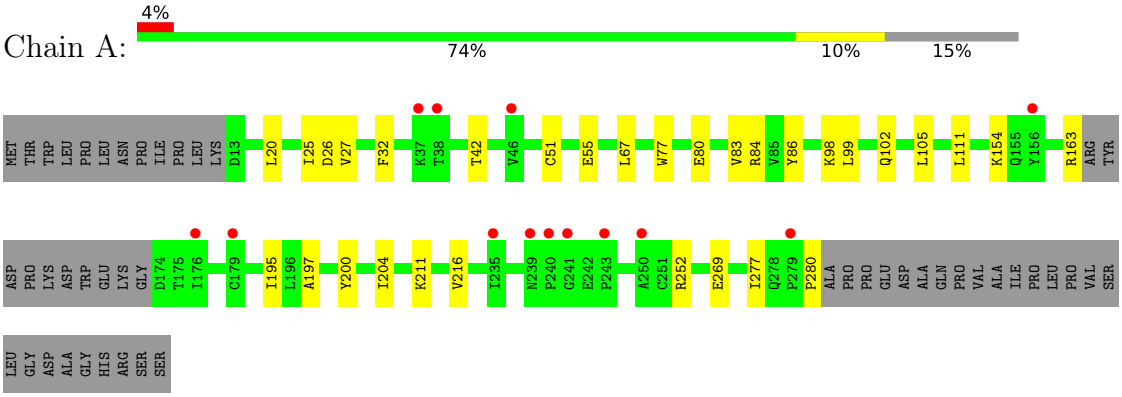
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	25	Total O 25 25	0	0
3	D	6	Total O 6 6	0	0
3	E	8	Total O 8 8	0	0
3	F	16	Total O 16 16	0	0

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.

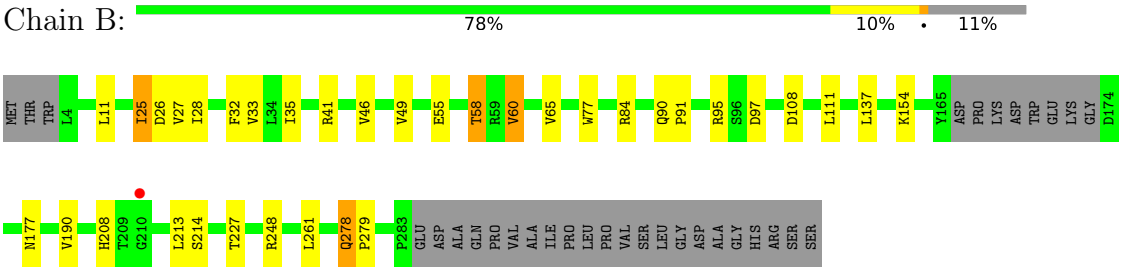
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain A:



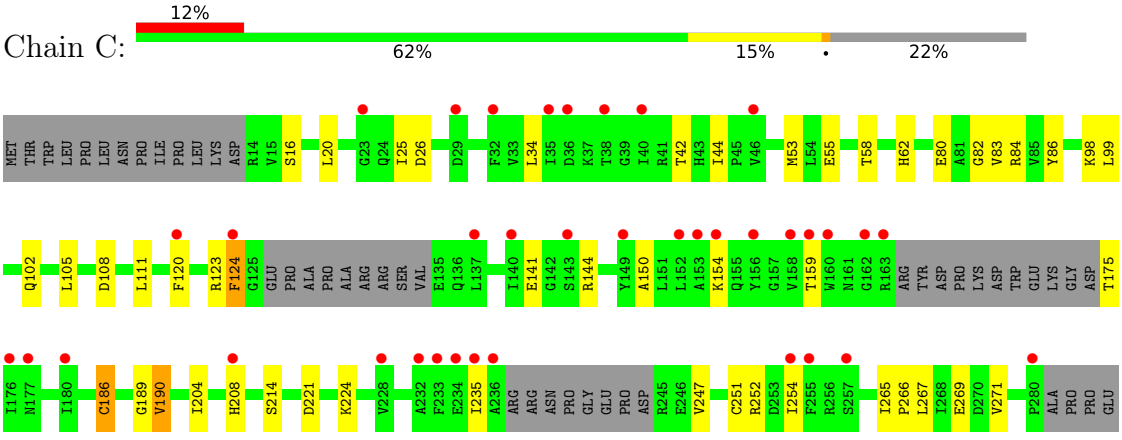
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain B:



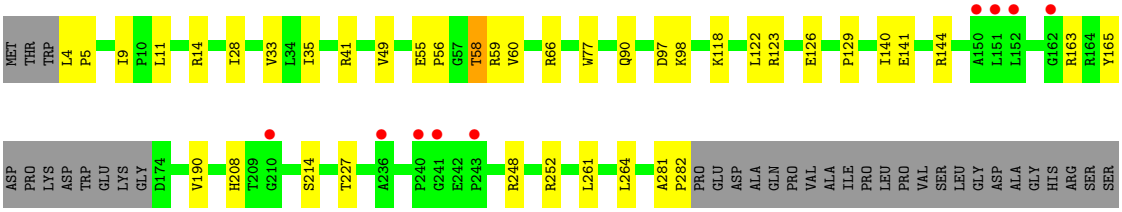
• Molecule 1: CRISPR-associated endonuclease Cas1

Chain C:



• Molecule 1: CRISPR-associated endonuclease Cas1

Chain D:

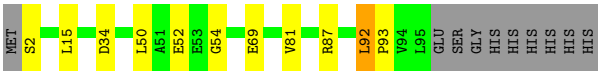


• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain E:

• Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.76Å 127.40Å 96.64Å 90.00° 100.89° 90.00°	Depositor
Resolution (Å)	47.45 – 2.70 47.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.45-2.70) 100.0 (47.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, R_{free}	0.227 , 0.261 0.229 , 0.261	Depositor DCC
R_{free} test set	5949 reflections (9.82%)	wwPDB-VP
Wilson B-factor (Å^2)	56.6	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9133	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/1850	0.50	0/2526
1	B	0.36	0/2093	0.52	0/2842
1	C	0.34	0/1729	0.49	0/2355
1	D	0.33	0/2070	0.49	0/2817
2	E	0.37	0/745	0.58	0/1014
2	F	0.37	0/740	0.54	0/1010
All	All	0.35	0/9227	0.51	0/12564

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	1817	0	1773	16	0
1	B	2071	0	2135	20	0
1	C	1702	0	1686	26	0
1	D	2030	0	2072	21	0
2	E	731	0	744	9	0
2	F	726	0	731	7	0
3	A	1	0	0	0	0
3	B	25	0	0	0	0
3	D	6	0	0	0	0
3	E	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	16	0	0	0	0
All	All	9133	0	9141	92	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 (92) 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:A:55:GLU:OE2	1:A:252:ARG:NH2	2.11	0.83
2:F:69:GLU:OE2	2:F:87:ARG:NH1	2.15	0.79
1:D:28:ILE:HD11	1:D:35:ILE:HD11	1.70	0.74
1:D:4:LEU:HD12	1:D:5:PRO:HD2	1.74	0.70
1:C:20:LEU:HD22	1:C:34:LEU:HD22	1.75	0.69
1:B:41:ARG:HG3	1:B:41:ARG:HH11	1.59	0.67
2:F:2:SER:N	2:F:34:ASP:OD1	2.27	0.67
1:A:84:ARG:NH1	1:A:86:TYR:OH	2.31	0.63
1:A:98:LYS:NZ	1:A:269:GLU:OE2	2.26	0.61
1:B:55:GLU:O	1:B:58:THR:OG1	2.18	0.61
1:C:98:LYS:NZ	1:C:269:GLU:OE2	2.32	0.60
1:C:251:CYS:HA	1:C:254:ILE:HD12	1.83	0.59
1:B:26:ASP:OD1	1:B:27:VAL:N	2.35	0.59
1:A:77:TRP:CD2	1:B:65:VAL:HG11	2.38	0.57
1:D:252:ARG:NE	2:E:65:GLU:OE2	2.37	0.57
1:B:84:ARG:HD3	1:B:213:LEU:HD11	1.87	0.57
1:C:123:ARG:HH11	1:C:141:GLU:HG2	1.70	0.55
1:B:25:ILE:HD13	1:B:60:VAL:HG13	1.89	0.55
1:D:60:VAL:HG11	1:D:77:TRP:HZ2	1.72	0.54
1:D:55:GLU:O	1:D:58:THR:OG1	2.24	0.54
1:C:124:PHE:HB3	1:C:144:ARG:NE	2.23	0.53
1:D:126:GLU:OE2	1:D:144:ARG:NH2	2.33	0.52
1:A:55:GLU:CD	1:A:252:ARG:HH22	2.13	0.52
1:C:221:ASP:HA	1:C:224:LYS:HD2	1.92	0.51
1:A:32:PHE:HD2	1:A:67:LEU:HD23	1.76	0.51
2:E:52:GLU:HG3	2:E:53:GLU:OE1	2.11	0.50
1:C:235:ILE:HD13	1:C:247:VAL:HA	1.93	0.49
1:D:123:ARG:NH1	1:D:141:GLU:OE2	2.45	0.49
1:D:208:HIS:O	1:D:214:SER:HB3	2.11	0.49
1:C:102:GLN:NE2	1:C:204:ILE:HB	2.28	0.49
1:B:208:HIS:O	1:B:214:SER:HB3	2.12	0.49
1:D:97:ASP:OD1	1:D:98:LYS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ARG:HD2	1:C:86:TYR:OH	2.13	0.48
1:A:20:LEU:HD13	1:A:25:ILE:HD12	1.96	0.48
1:B:278:GLN:HA	1:B:279:PRO:HD3	1.71	0.48
1:A:51:CYS:HB2	1:A:197:ALA:HB2	1.95	0.48
1:B:190:VAL:HB	1:B:261:LEU:HD21	1.96	0.47
1:C:34:LEU:HB2	1:C:44:ILE:HD11	1.96	0.47
1:B:32:PHE:CG	1:B:46:VAL:HB	2.49	0.47
2:E:69:GLU:OE2	2:E:87:ARG:NE	2.40	0.47
1:A:98:LYS:HD3	1:A:280:PRO:HG2	1.97	0.47
2:E:14:ARG:HG2	2:E:50:LEU:HD13	1.96	0.47
2:E:81:VAL:HG21	2:E:90:SER:OG	2.15	0.47
1:A:195:ILE:HG23	1:A:200:TYR:HB2	1.97	0.47
1:A:211:LYS:HA	1:A:211:LYS:HD2	1.78	0.46
1:A:80:GLU:O	1:A:83:VAL:HG23	2.16	0.46
1:B:28:ILE:HD11	1:B:35:ILE:HD11	1.97	0.46
1:B:95:ARG:HB3	1:B:97:ASP:OD1	2.16	0.46
1:C:108:ASP:OD2	1:C:111:LEU:HG	2.16	0.46
1:D:55:GLU:OE2	1:D:248:ARG:NH1	2.44	0.45
1:D:190:VAL:HB	1:D:261:LEU:HD21	1.98	0.45
1:B:41:ARG:HH11	1:B:41:ARG:CG	2.29	0.45
1:D:163:ARG:HG2	1:D:165:TYR:CZ	2.51	0.45
2:E:2:SER:OG	2:E:61:ALA:O	2.27	0.45
1:D:41:ARG:HH12	2:E:94:VAL:H	1.64	0.45
1:C:55:GLU:OE1	1:C:252:ARG:NH2	2.50	0.45
1:C:62:HIS:CG	1:D:56:PRO:HA	2.53	0.44
1:D:118:LYS:HE3	1:D:122:LEU:HD11	1.99	0.44
1:A:105:LEU:HD23	1:A:111:LEU:HD13	1.99	0.44
1:B:137:LEU:HA	1:B:137:LEU:HD23	1.72	0.44
1:B:108:ASP:OD2	1:B:111:LEU:HG	2.18	0.44
1:D:264:LEU:HA	1:D:264:LEU:HD23	1.85	0.44
1:C:150:ALA:O	1:C:154:LYS:HG2	2.18	0.44
1:C:120:PHE:HB3	1:C:124:PHE:CZ	2.52	0.44
1:C:26:ASP:OD2	1:D:59:ARG:NH2	2.51	0.43
1:D:9:ILE:HG13	1:D:14:ARG:HE	1.81	0.43
1:B:55:GLU:OE2	1:B:248:ARG:NH1	2.51	0.43
1:B:90[B]:GLN:HA	1:B:91:PRO:HD3	1.83	0.43
1:C:265:ILE:HB	1:C:266:PRO:HD3	2.00	0.42
1:C:267:LEU:O	1:C:271:VAL:HG23	2.19	0.42
2:F:92:LEU:HD12	2:F:92:LEU:HA	1.80	0.42
1:D:129:PRO:HG2	1:D:140:ILE:HD13	2.02	0.42
2:F:15:LEU:HD13	2:F:50:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:GLY:O	1:C:189:GLY:HA3	2.20	0.42
1:C:80:GLU:O	1:C:83:VAL:HG23	2.20	0.42
1:A:195:ILE:HD12	1:A:216:VAL:HG22	2.01	0.41
2:E:23:LEU:HB2	2:E:31:TYR:HB3	2.02	0.41
1:B:28:ILE:CD1	1:B:35:ILE:HD11	2.51	0.41
1:B:41:ARG:NH1	2:F:93:PRO:HG3	2.36	0.41
1:C:235:ILE:HD13	1:C:247:VAL:HG22	2.01	0.41
2:E:79:THR:HA	2:E:80:PRO:HD2	1.81	0.41
1:A:102:GLN:NE2	1:A:204:ILE:HB	2.36	0.41
2:F:52:GLU:C	2:F:54:GLY:H	2.23	0.41
1:A:26:ASP:OD1	1:A:27:VAL:N	2.51	0.41
1:C:53:MET:SD	1:C:190:VAL:HG12	2.61	0.41
2:F:81:VAL:O	2:F:87:ARG:HD3	2.21	0.41
1:C:105:LEU:HD23	1:C:111:LEU:HD13	2.02	0.41
1:D:281:ALA:HA	1:D:282:PRO:HD3	1.85	0.41
1:C:86:TYR:CE1	1:D:66:ARG:HD2	2.56	0.40
1:B:60:VAL:HG21	1:B:77:TRP:CZ2	2.56	0.40
1:C:186:CYS:O	1:C:190:VAL:HG22	2.21	0.40
1:C:208:HIS:O	1:C:214:SER:HB3	2.21	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	254/305 (83%)	246 (97%)	8 (3%)	0	100	100
1	B	269/305 (88%)	266 (99%)	3 (1%)	0	100	100
1	C	231/305 (76%)	228 (99%)	3 (1%)	0	100	100
1	D	267/305 (88%)	263 (98%)	4 (2%)	0	100	100
2	E	91/104 (88%)	90 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	92/104 (88%)	90 (98%)	2 (2%)	0	100	100
All	All	1204/1428 (84%)	1183 (98%)	21 (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	166/245 (68%)	161 (97%)	5 (3%)	41	70
1	B	211/245 (86%)	201 (95%)	10 (5%)	26	54
1	C	159/245 (65%)	149 (94%)	10 (6%)	18	40
1	D	205/245 (84%)	199 (97%)	6 (3%)	42	71
2	E	78/88 (89%)	75 (96%)	3 (4%)	33	62
2	F	76/88 (86%)	75 (99%)	1 (1%)	69	87
All	All	895/1156 (77%)	860 (96%)	35 (4%)	32	61

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	THR
1	A	99	LEU
1	A	154	LYS
1	A	163	ARG
1	A	277	ILE
1	B	11	LEU
1	B	25	ILE
1	B	33	VAL
1	B	49	VAL
1	B	58	THR
1	B	60	VAL
1	B	154	LYS
1	B	177	ASN

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Mol	Chain	Res	Type
1	B	227	THR
1	B	278	GLN
1	C	16	SER
1	C	25	ILE
1	C	42	THR
1	C	58	THR
1	C	99	LEU
1	C	124	PHE
1	C	159	THR
1	C	175	THR
1	C	186	CYS
1	C	190	VAL
1	D	11	LEU
1	D	33	VAL
1	D	49	VAL
1	D	58	THR
1	D	90	GLN
1	D	227	THR
2	E	52	GLU
2	E	63	ASN
2	E	65	GLU
2	F	92	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	10	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

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	258/305 (84%)	0.23	13 (5%) 28 27	48, 73, 99, 108	0
1	B	272/305 (89%)	-0.03	1 (0%) 92 93	40, 57, 86, 115	0
1	C	239/305 (78%)	0.63	37 (15%) 2 1	52, 74, 100, 124	0
1	D	271/305 (88%)	0.06	9 (3%) 46 46	42, 58, 88, 99	0
2	E	93/104 (89%)	-0.27	0 100 100	37, 50, 68, 78	1 (1%)
2	F	94/104 (90%)	-0.24	0 100 100	38, 48, 66, 80	1 (1%)
All	All	1227/1428 (85%)	0.14	60 (4%) 29 28	37, 63, 95, 124	2 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	235	ILE	6.1
1	C	158	VAL	5.3
1	C	233	PHE	5.1
1	C	40	ILE	4.7
1	B	210	GLY	4.4
1	C	236	ALA	4.4
1	D	210	GLY	4.2
1	A	240	PRO	3.9
1	A	38	THR	3.8
1	C	159	THR	3.8
1	C	160	TRP	3.5
1	C	140	ILE	3.4
1	C	137	LEU	3.3
1	C	152	LEU	3.3
1	C	176	ILE	3.2
1	A	46	VAL	3.2
1	C	143	SER	3.2
1	C	46	VAL	3.1
1	C	232	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	254	ILE	3.1
1	A	241	GLY	3.0
1	C	257	SER	3.0
1	A	243	PRO	3.0
1	D	240	PRO	3.0
1	C	153	ALA	2.9
1	C	156	TYR	2.9
1	C	177	ASN	2.8
1	D	241	GLY	2.8
1	C	180	ILE	2.8
1	C	234	GLU	2.7
1	C	255	PHE	2.7
1	C	124	PHE	2.6
1	C	162	GLY	2.6
1	A	279	PRO	2.6
1	C	280	PRO	2.6
1	D	150	ALA	2.5
1	C	154	LYS	2.5
1	C	35	ILE	2.5
1	C	149	TYR	2.5
1	C	208	HIS	2.5
1	C	32	PHE	2.5
1	D	243	PRO	2.4
1	C	120	PHE	2.4
1	A	239	ASN	2.4
1	A	179	CYS	2.3
1	C	29	ASP	2.3
1	A	176	ILE	2.3
1	A	250	ALA	2.3
1	C	23	GLY	2.2
1	C	228	VAL	2.2
1	A	235	ILE	2.2
1	D	162	GLY	2.2
1	C	38	THR	2.2
1	C	163	ARG	2.1
1	C	36	ASP	2.1
1	A	37	LYS	2.1
1	A	156	TYR	2.1
1	D	152	LEU	2.0
1	D	236	ALA	2.0
1	D	151	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.