



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID : 1IU3
Title : CRYSTAL STRUCTURE OF THE E.COLI SEQA PROTEIN COMPLEXED WITH HEMIMETHYLATED DNA
Authors : Fujikawa, N.; Kurumizaka, H.; Nureki, O.; Tanaka, Y.; Yamazoe, M.; Hiraga, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-02-26
Resolution : 3.00 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

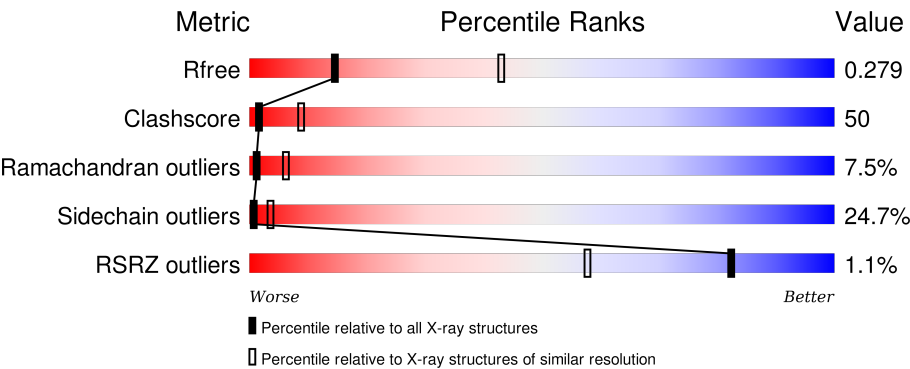
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 $\leq 5\%$. 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	10	<div><div></div><div><div></div><div>30%</div><div>30%</div><div>20%</div><div>20%</div></div></div>
1	D	10	<div><div></div><div><div></div><div>10%</div><div>60%</div><div>20%</div><div>10%</div></div></div>
2	B	10	<div><div></div><div><div></div><div>20%</div><div>70%</div><div>10%</div></div></div>
2	E	10	<div><div></div><div><div></div><div>10%</div><div>60%</div><div>40%</div></div></div>
3	C	116	<div><div></div><div><div></div><div>%</div><div>21%</div><div>47%</div><div>20%</div><div>11%</div><div>.</div></div></div>

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Mol	Chain	Length	Quality of chain
3	F	116	<div><div><div></div><div></div><div></div><div></div></div><div>%27%47%21%5%•</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2755 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 DNA chain called 5'-D(*AP*AP*GP*GP*AP*TP*CP*CP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	10	Total	C	N	O	P	0	0	0
			204	98	43	54	9			
1	D	10	Total	C	N	O	P	0	0	0
			204	98	43	54	9			

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*GP*GP*AP*TP*CP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	P	0	0	0
			200	98	31	62	9			
2	E	10	Total	C	N	O	P	0	0	0
			200	98	31	62	9			

- Molecule 3 is a protein called SeqA protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	115	Total	C	N	O	S	0	0	0
			908	572	157	172	7			
3	F	115	Total	C	N	O	S	0	0	0
			908	572	157	172	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	CLONING ARTIFACT	UNP P36658
C	2	PRO	-	CLONING ARTIFACT	UNP P36658
C	3	LEU	-	CLONING ARTIFACT	UNP P36658
C	4	GLY	-	CLONING ARTIFACT	UNP P36658
C	5	SER	-	CLONING ARTIFACT	UNP P36658
F	1	GLY	-	CLONING ARTIFACT	UNP P36658
F	2	PRO	-	CLONING ARTIFACT	UNP P36658
F	3	LEU	-	CLONING ARTIFACT	UNP P36658

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4	GLY	-	CLONING ARTIFACT	UNP P36658
F	5	SER	-	CLONING ARTIFACT	UNP P36658


- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total O 9 9	0	0
4	B	9	Total O 9 9	0	0
4	C	59	Total O 59 59	0	0
4	D	12	Total O 12 12	0	0
4	E	13	Total O 13 13	0	0
4	F	29	Total O 29 29	0	0

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.

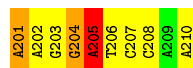
- Molecule 1: 5'-D(*AP*AP*GP*GP*AP*TP*CP*CP*AP*A)-3'

Chain A: 



- Molecule 1: 5'-D(*AP*AP*GP*GP*AP*TP*CP*CP*AP*A)-3'

Chain D: 



- Molecule 2: 5'-D(*TP*TP*GP*GP*AP*TP*CP*CP*TP*T)-3'

Chain B: 




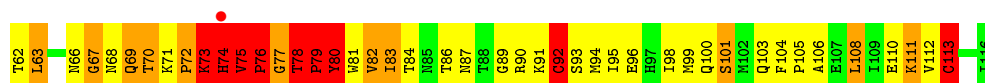
- Molecule 2: 5'-D(*TP*TP*GP*GP*AP*TP*CP*CP*TP*T)-3'

Chain E: 

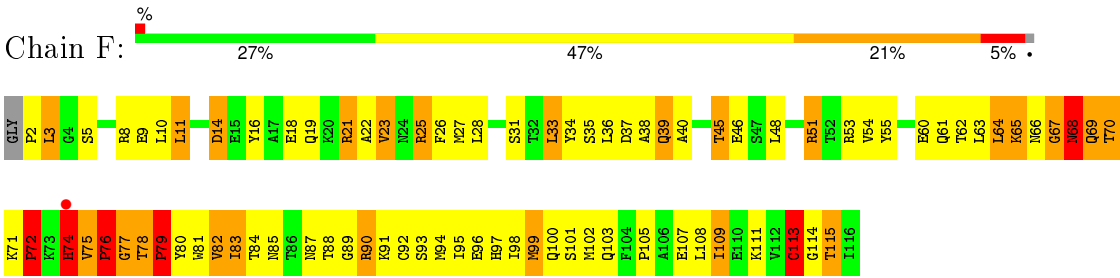


- Molecule 3: SeqA protein

Chain C: 



- Molecule 3: SeqA protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 6 2 2	Depositor
Cell constants a, b, c, α , β , γ	152.59 Å 152.59 Å 119.36 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.00 41.33 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.8 (41.33-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 3.01 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.286 0.237 , 0.279	Depositor DCC
R_{free} test set	816 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	85.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 16587 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2755	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	2.05	9/230 (3.9%)	1.96	11/353 (3.1%)
1	D	1.69	5/230 (2.2%)	1.60	4/353 (1.1%)
2	B	1.94	5/222 (2.3%)	1.77	7/341 (2.1%)
2	E	1.46	0/222	1.46	2/341 (0.6%)
3	C	2.02	22/925 (2.4%)	1.83	30/1248 (2.4%)
3	F	1.29	4/925 (0.4%)	1.39	8/1248 (0.6%)
All	All	1.73	45/2754 (1.6%)	1.66	62/3884 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
2	B	0	3
2	E	0	3
3	C	0	2
All	All	0	12

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	75	VAL	CA-CB	11.86	1.79	1.54
3	C	16	TYR	CE2-CZ	-9.64	1.26	1.38
3	F	113	CYS	CB-SG	9.17	1.97	1.82
3	C	23	VAL	CB-CG2	-8.37	1.35	1.52
3	C	92	CYS	CB-SG	-7.78	1.69	1.82
1	A	204	DG	N3-C4	-7.59	1.30	1.35
1	A	204	DG	N7-C5	-7.55	1.34	1.39
3	C	5	SER	CB-OG	7.42	1.51	1.42
3	C	9	GLU	CG-CD	7.33	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	204	DG	N9-C4	-7.19	1.32	1.38
3	F	76	PRO	CA-C	6.50	1.65	1.52
3	C	16	TYR	CE1-CZ	-6.48	1.30	1.38
2	B	215	DA	N1-C2	-6.47	1.28	1.34
2	B	211	DT	O3'-P	6.46	1.68	1.61
3	C	80	TYR	CB-CG	-6.44	1.42	1.51
1	A	204	DG	N9-C8	-6.44	1.33	1.37
3	C	43	GLU	CG-CD	6.33	1.61	1.51
3	C	106	ALA	CA-CB	-6.30	1.39	1.52
3	F	75	VAL	CA-CB	6.28	1.68	1.54
3	C	76	PRO	CB-CG	6.16	1.80	1.50
3	C	15	GLU	CG-CD	6.03	1.60	1.51
1	A	203	DG	N9-C8	-5.96	1.33	1.37
2	B	215	DA	C5-C4	-5.96	1.34	1.38
1	A	210	DA	C5-C6	-5.91	1.35	1.41
2	B	220	DT	C4-C5	5.89	1.50	1.45
1	A	204	DG	C3'-O3'	-5.89	1.36	1.44
1	D	204	DG	N9-C4	-5.82	1.33	1.38
1	D	204	DG	C5-C6	-5.79	1.36	1.42
1	A	203	DG	N7-C5	-5.71	1.35	1.39
3	C	15	GLU	CD-OE2	5.67	1.31	1.25
3	F	39	GLN	CG-CD	5.61	1.64	1.51
3	C	46	GLU	CD-OE1	5.60	1.31	1.25
1	D	201	DA	C2'-C1'	5.52	1.57	1.52
3	C	101	SER	CB-OG	5.52	1.49	1.42
3	C	75	VAL	CB-CG2	-5.52	1.41	1.52
2	B	214	DG	C5-C6	-5.45	1.36	1.42
1	D	204	DG	N3-C4	-5.42	1.31	1.35
3	C	9	GLU	CD-OE1	5.29	1.31	1.25
3	C	43	GLU	CD-OE1	5.17	1.31	1.25
3	C	61	GLN	CG-CD	5.13	1.62	1.51
1	A	202	DA	N1-C2	5.11	1.39	1.34
3	C	19	GLN	CG-CD	-5.10	1.39	1.51
3	C	110	GLU	CD-OE2	5.06	1.31	1.25
1	D	201	DA	O3'-P	5.06	1.67	1.61
3	C	20	LYS	CB-CG	5.03	1.66	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	DG	O5'-P-OP2	-13.65	93.42	105.70
1	D	202	DA	O5'-P-OP2	-12.14	94.78	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	75	VAL	C-N-CD	-10.59	97.30	120.60
3	C	25	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	A	203	DG	O5'-P-OP1	9.52	122.12	110.70
2	B	212	DT	O5'-P-OP1	-9.05	97.56	105.70
1	A	205	DA	C5'-C4'-C3'	-8.76	98.34	114.10
3	C	70	THR	N-CA-C	-8.31	88.56	111.00
3	F	70	THR	N-CA-C	-7.68	90.27	111.00
3	C	73	LYS	CA-C-N	-7.66	100.36	117.20
3	C	23	VAL	CB-CA-C	-7.52	97.11	111.40
3	C	11	LEU	CA-CB-CG	7.43	132.38	115.30
3	C	75	VAL	N-CA-C	-7.31	91.26	111.00
1	A	202	DA	O5'-P-OP1	-7.31	99.12	105.70
3	C	11	LEU	CB-CG-CD2	-7.30	98.59	111.00
3	C	25	ARG	NE-CZ-NH2	7.21	123.90	120.30
3	C	74	HIS	N-CA-C	7.07	130.09	111.00
3	F	82	VAL	CB-CA-C	-7.01	98.08	111.40
1	D	201	DA	N9-C1'-C2'	6.99	125.89	112.60
3	F	68	ASN	N-CA-C	6.73	129.17	111.00
1	A	204	DG	O5'-P-OP2	-6.70	99.67	105.70
3	F	21	ARG	NE-CZ-NH2	-6.69	116.95	120.30
3	C	69	GLN	N-CA-C	-6.66	93.03	111.00
2	E	212	DT	O5'-P-OP1	-6.64	99.72	105.70
3	C	74	HIS	C-N-CA	-6.59	105.23	121.70
3	C	73	LYS	CA-C-O	6.50	133.75	120.10
3	C	76	PRO	N-CA-CB	-6.49	95.46	102.60
3	C	70	THR	C-N-CA	-6.47	105.53	121.70
2	B	212	DT	OP1-P-O3'	6.26	118.97	105.20
3	C	82	VAL	CB-CA-C	-6.21	99.60	111.40
3	C	68	ASN	N-CA-C	6.19	127.72	111.00
1	A	202	DA	C5'-C4'-C3'	-6.05	103.20	114.10
2	B	211	DT	N1-C1'-C2'	6.03	124.06	112.60
1	A	204	DG	OP1-P-O3'	6.00	118.40	105.20
3	C	63	LEU	CB-CG-CD1	-5.94	100.90	111.00
3	C	78	THR	CA-CB-CG2	-5.86	104.20	112.40
1	D	205	DA	C5'-C4'-C3'	-5.81	103.64	114.10
3	F	33	LEU	CA-CB-CG	5.77	128.56	115.30
2	B	213	DG	O4'-C4'-C3'	5.75	109.45	106.00
3	C	21	ARG	NE-CZ-NH2	-5.71	117.44	120.30
3	C	113	CYS	CA-CB-SG	-5.64	103.84	114.00
3	C	33	LEU	CA-CB-CG	5.62	128.23	115.30
3	C	68	ASN	C-N-CA	-5.57	107.77	121.70
3	F	11	LEU	CA-CB-CG	5.52	128.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	208	DC	C1'-O4'-C4'	-5.49	104.61	110.10
2	B	211	DT	O4'-C1'-N1	5.38	111.77	108.00
1	A	204	DG	O4'-C1'-C2'	-5.36	101.61	105.90
2	E	214	DG	O4'-C1'-N9	-5.33	104.27	108.00
3	C	111	LYS	CB-CG-CD	5.29	125.36	111.60
2	B	214	DG	OP2-P-O3'	5.23	116.70	105.20
3	C	59	ASP	CB-CG-OD2	5.22	123.00	118.30
3	C	92	CYS	CA-CB-SG	-5.21	104.63	114.00
1	A	202	DA	OP2-P-O3'	5.16	116.56	105.20
3	C	83	ILE	CG1-CB-CG2	-5.16	100.04	111.40
1	A	201	DA	OP2-P-O3'	5.14	116.50	105.20
1	A	204	DG	C2'-C3'-O3'	-5.08	95.82	112.60
3	C	78	THR	N-CA-CB	-5.07	100.66	110.30
3	C	80	TYR	CB-CG-CD2	-5.07	117.96	121.00
3	F	25	ARG	NE-CZ-NH2	5.07	122.83	120.30
3	C	29	LEU	CB-CG-CD2	-5.04	102.43	111.00
2	B	219	DT	N1-C1'-C2'	-5.03	103.04	112.60
3	F	21	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	DA	Sidechain
1	A	210	DA	Sidechain
2	B	211	DT	Sidechain
2	B	217	DC	Sidechain
2	B	220	DT	Sidechain
3	C	75	VAL	Mainchain
3	C	80	TYR	Sidechain
1	D	205	DA	Sidechain
1	D	210	DA	Sidechain
2	E	211	DT	Sidechain
2	E	216	DT	Sidechain
2	E	219	DT	Sidechain

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	204	0	113	7	0
1	D	204	0	113	10	4
2	B	200	0	117	17	0
2	E	200	0	117	14	0
3	C	908	0	909	98	0
3	F	908	0	909	108	0
4	A	9	0	0	4	0
4	B	9	0	0	4	0
4	C	59	0	0	21	0
4	D	12	0	0	4	0
4	E	13	0	0	7	0
4	F	29	0	0	12	0
All	All	2755	0	2278	243	4

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 50.

All (243) 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:C:75:VAL:CA	3:C:75:VAL:CB	1.79	1.55
3:F:27:MET:SD	3:F:27:MET:CE	2.03	1.46
3:C:76:PRO:CB	3:C:76:PRO:CG	1.80	1.45
3:C:113:CYS:HB2	4:C:174:HOH:O	1.46	1.14
3:F:77:GLY:HA2	4:F:126:HOH:O	1.47	1.12
3:C:61:GLN:HG3	4:C:121:HOH:O	1.52	1.10
2:B:211:DT:H2'	4:B:9:HOH:O	1.68	0.94
3:C:89:GLY:O	3:C:92:CYS:HB2	1.69	0.92
4:D:78:HOH:O	3:F:87:ASN:HB2	1.68	0.90
3:F:96:GLU:HG2	3:F:100:GLN:NE2	1.87	0.89
3:F:26:PHE:CD1	3:F:91:LYS:HG3	2.06	0.89
2:E:215:DA:H2''	2:E:216:DT:H72	1.55	0.88
3:C:21:ARG:HB2	3:C:24:ASN:ND2	1.89	0.88
3:F:19:GLN:OE1	3:F:19:GLN:HA	1.73	0.88
3:C:9:GLU:HB3	4:C:136:HOH:O	1.74	0.88
1:D:203:DG:H4'	3:F:21:ARG:NH1	1.88	0.87
3:C:103:GLN:HA	4:C:129:HOH:O	1.73	0.86
3:F:99:MET:HB3	3:F:109:ILE:CD1	2.06	0.85
3:C:3:LEU:HA	4:C:118:HOH:O	1.76	0.84
4:B:123:HOH:O	3:C:67:GLY:HA2	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:TYR:HA	3:C:83:ILE:HG12	1.58	0.83
3:F:3:LEU:HA	4:F:135:HOH:O	1.77	0.83
3:C:21:ARG:HB2	3:C:24:ASN:HD22	1.43	0.82
3:F:51:ARG:HG3	3:F:51:ARG:HH11	1.45	0.82
2:E:213:DG:H5''	4:E:30:HOH:O	1.79	0.81
3:F:79:PRO:HG2	3:F:80:TYR:CD1	2.17	0.80
3:F:68:ASN:HD22	3:F:69:GLN:H	1.29	0.79
3:F:51:ARG:CG	3:F:51:ARG:HH11	1.95	0.78
2:E:213:DG:N3	4:E:101:HOH:O	2.17	0.78
3:F:61:GLN:HG3	4:F:121:HOH:O	1.82	0.78
3:C:96:GLU:O	3:C:100:GLN:HG3	1.86	0.76
2:E:215:DA:H2''	2:E:216:DT:C7	2.15	0.76
1:D:204:DG:OP2	3:F:23:VAL:HG23	1.85	0.75
1:D:206:DT:H2''	1:D:207:DC:C6	2.21	0.75
3:C:73:LYS:HG3	3:C:74:HIS:CE1	2.20	0.75
3:C:66:ASN:HB3	4:C:125:HOH:O	1.86	0.75
3:F:94:MET:O	3:F:98:ILE:HG13	1.86	0.74
3:C:11:LEU:HB3	4:C:155:HOH:O	1.87	0.74
3:C:75:VAL:CG1	3:C:75:VAL:CA	2.66	0.73
3:F:79:PRO:HG2	3:F:80:TYR:CE1	2.23	0.73
3:C:78:THR:HG22	4:C:144:HOH:O	1.88	0.72
3:C:90:ARG:O	3:C:94:MET:HG3	1.90	0.72
3:F:68:ASN:HD22	3:F:69:GLN:N	1.88	0.71
2:E:211:DT:H2''	4:E:90:HOH:O	1.90	0.70
3:F:71:LYS:HB2	3:F:84:THR:HB	1.74	0.70
3:F:68:ASN:O	4:F:119:HOH:O	2.10	0.70
3:F:5:SER:HB2	4:F:117:HOH:O	1.92	0.69
2:B:211:DT:H5'	4:E:29:HOH:O	1.92	0.69
3:F:78:THR:HB	3:F:79:PRO:CD	2.23	0.69
3:C:78:THR:HA	4:C:144:HOH:O	1.94	0.68
2:B:211:DT:C2'	4:B:9:HOH:O	2.33	0.68
3:C:75:VAL:CB	3:C:75:VAL:HA	2.15	0.67
3:F:99:MET:HE2	3:F:109:ILE:HD13	1.75	0.67
2:B:215:DA:H2''	2:B:216:DT:H72	1.77	0.67
3:F:107:GLU:HG2	3:F:111:LYS:NZ	2.10	0.67
3:C:74:HIS:CE1	4:C:141:HOH:O	2.47	0.67
3:C:113:CYS:CB	4:C:174:HOH:O	2.16	0.67
3:F:53:ARG:HG2	3:F:67:GLY:HA3	1.77	0.67
3:C:94:MET:O	3:C:98:ILE:HG13	1.94	0.66
2:B:211:DT:H71	4:D:69:HOH:O	1.96	0.66
3:C:75:VAL:CA	3:C:75:VAL:CG2	2.68	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:108:LEU:O	3:F:111:LYS:HB2	1.95	0.66
3:C:108:LEU:O	3:C:111:LYS:HB2	1.97	0.65
3:F:99:MET:HB3	3:F:109:ILE:HD11	1.78	0.65
3:F:11:LEU:HD12	3:F:115:THR:HG21	1.79	0.65
3:C:83:ILE:N	3:C:83:ILE:HD13	2.10	0.64
3:F:83:ILE:HD13	3:F:83:ILE:N	2.12	0.64
1:D:203:DG:H4'	3:F:21:ARG:HH11	1.60	0.64
3:F:78:THR:HB	3:F:79:PRO:HD2	1.77	0.64
2:B:219:DT:OP1	2:B:219:DT:H4'	1.98	0.64
3:C:53:ARG:NH2	3:C:69:GLN:O	2.32	0.63
3:C:2:PRO:HD3	3:C:105:PRO:HD3	1.80	0.62
3:C:63:LEU:HD22	3:C:83:ILE:HD11	1.81	0.62
3:F:51:ARG:NH1	3:F:51:ARG:HB2	2.14	0.62
3:F:53:ARG:NE	3:F:70:THR:HG22	2.15	0.61
3:F:92:CYS:HB2	4:F:141:HOH:O	2.00	0.61
3:C:61:GLN:O	3:C:62:THR:C	2.35	0.61
3:C:75:VAL:C	3:C:75:VAL:CB	2.67	0.61
3:F:96:GLU:HG2	3:F:100:GLN:HE22	1.65	0.61
3:C:48:LEU:HD21	3:C:94:MET:HB3	1.82	0.61
3:C:5:SER:O	3:C:9:GLU:HG3	2.02	0.60
3:F:111:LYS:O	3:F:114:GLY:N	2.35	0.60
3:F:96:GLU:HG2	3:F:100:GLN:HE21	1.65	0.59
3:F:51:ARG:NH1	3:F:51:ARG:CB	2.65	0.59
3:C:71:LYS:C	4:C:135:HOH:O	2.40	0.59
3:F:99:MET:HB3	3:F:109:ILE:HD13	1.85	0.59
3:F:89:GLY:O	3:F:92:CYS:HB3	2.03	0.59
3:F:55:TYR:HA	3:F:83:ILE:HG12	1.84	0.59
3:C:8:ARG:HA	3:C:11:LEU:HD23	1.84	0.59
1:A:205:DA:H2''	1:A:206:DT:C6	2.37	0.59
3:F:25:ARG:HG3	3:F:25:ARG:HH11	1.67	0.59
3:C:48:LEU:HD23	3:C:56:PHE:HE1	1.67	0.58
3:C:7:MET:O	3:C:11:LEU:CD2	2.51	0.58
3:F:69:GLN:HA	3:F:69:GLN:HE21	1.68	0.58
3:F:107:GLU:HG2	3:F:111:LYS:HZ1	1.69	0.58
3:C:11:LEU:HD11	3:C:112:VAL:HG22	1.85	0.58
3:C:3:LEU:HD23	3:C:3:LEU:H	1.68	0.57
3:F:60:GLU:HG2	3:F:64:LEU:CD1	2.34	0.57
3:C:86:THR:OG1	3:C:91:LYS:HE2	2.05	0.56
3:C:77:GLY:O	4:C:144:HOH:O	2.17	0.55
3:F:51:ARG:NH1	3:F:51:ARG:CG	2.62	0.55
3:F:60:GLU:HG2	3:F:64:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:LEU:O	3:C:13:SER:OG	2.25	0.54
3:C:7:MET:O	3:C:11:LEU:HD22	2.08	0.54
3:C:27:MET:HE1	3:C:76:PRO:HD3	1.90	0.54
1:A:205:DA:N7	3:C:87:ASN:HB3	2.22	0.54
3:F:64:LEU:HG	3:F:72:PRO:HG2	1.90	0.54
3:F:55:TYR:OH	3:F:90:ARG:HD3	2.08	0.54
3:F:45:THR:HG22	3:F:46:GLU:N	2.21	0.54
3:C:61:GLN:CG	4:C:121:HOH:O	2.29	0.53
3:F:61:GLN:O	3:F:62:THR:C	2.45	0.53
2:B:217:DC:H1'	2:B:218:DC:C6	2.43	0.53
3:C:56:PHE:CZ	3:C:98:ILE:HD11	2.44	0.53
1:A:204:DG:H2''	1:A:205:DA:C8	2.43	0.53
3:C:3:LEU:CD2	3:C:3:LEU:H	2.22	0.53
2:B:217:DC:H1'	2:B:218:DC:C5	2.44	0.53
2:E:216:DT:H2'	2:E:217:DC:C6	2.44	0.52
3:C:14:ASP:N	3:C:14:ASP:OD1	2.31	0.52
2:E:216:DT:H1'	4:E:128:HOH:O	2.09	0.52
3:F:78:THR:CB	3:F:79:PRO:CD	2.87	0.52
3:F:9:GLU:HB3	4:F:132:HOH:O	2.10	0.52
3:C:95:ILE:O	3:C:99:MET:HB2	2.09	0.52
3:F:98:ILE:HG22	3:F:98:ILE:O	2.10	0.52
3:C:11:LEU:N	3:C:11:LEU:HD22	2.24	0.52
3:F:23:VAL:O	3:F:26:PHE:HB3	2.10	0.52
1:D:204:DG:OP2	3:F:22:ALA:HB3	2.09	0.52
3:F:70:THR:C	3:F:72:PRO:HD3	2.31	0.51
3:C:89:GLY:O	3:C:92:CYS:CB	2.53	0.51
2:E:213:DG:H1'	4:E:101:HOH:O	2.09	0.51
3:C:71:LYS:O	3:C:72:PRO:C	2.48	0.51
3:F:91:LYS:NZ	4:F:140:HOH:O	2.43	0.51
3:C:48:LEU:HD23	3:C:56:PHE:CE1	2.46	0.51
3:F:27:MET:HE1	3:F:76:PRO:HD3	1.92	0.50
3:F:70:THR:OG1	3:F:72:PRO:HD3	2.11	0.50
3:F:63:LEU:HD13	3:F:83:ILE:HD13	1.92	0.50
3:C:33:LEU:O	3:C:34:TYR:C	2.49	0.50
2:B:214:DG:H1'	2:B:215:DA:H5'	1.93	0.50
3:F:51:ARG:HH11	3:F:51:ARG:CB	2.23	0.50
3:F:102:MET:O	3:F:103:GLN:HB2	2.12	0.50
3:F:70:THR:O	3:F:72:PRO:HD3	2.12	0.49
3:F:80:TYR:CD1	3:F:80:TYR:N	2.80	0.49
3:F:2:PRO:HD3	3:F:105:PRO:HD2	1.94	0.49
4:A:94:HOH:O	2:B:219:DT:C7	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:LEU:HG	3:C:55:TYR:HD2	1.77	0.49
3:F:19:GLN:OE1	3:F:19:GLN:CA	2.43	0.49
3:F:70:THR:O	3:F:72:PRO:CD	2.60	0.49
3:C:19:GLN:OE1	3:C:19:GLN:CA	2.56	0.49
3:C:41:PHE:O	3:C:44:ALA:HB3	2.13	0.49
1:D:206:DT:C2'	1:D:207:DC:C6	2.95	0.48
3:C:80:TYR:CD1	3:C:80:TYR:N	2.80	0.48
4:D:78:HOH:O	3:F:88:THR:N	2.46	0.48
3:C:74:HIS:HA	3:C:81:TRP:CZ3	2.48	0.48
3:C:100:GLN:O	3:C:101:SER:C	2.51	0.48
3:F:79:PRO:HG2	3:F:80:TYR:HD1	1.70	0.48
3:F:53:ARG:NH2	3:F:69:GLN:O	2.47	0.48
3:C:23:VAL:HG22	4:C:151:HOH:O	2.13	0.47
3:C:74:HIS:O	3:C:75:VAL:HG22	2.14	0.47
1:A:201:DA:H8	4:A:43:HOH:O	1.97	0.47
3:F:14:ASP:N	3:F:14:ASP:OD1	2.33	0.47
3:C:28:LEU:O	3:C:28:LEU:CD2	2.63	0.47
3:F:63:LEU:HB3	3:F:83:ILE:HD11	1.94	0.47
3:C:34:TYR:CD2	3:C:78:THR:CG2	2.98	0.47
3:C:21:ARG:CZ	4:C:122:HOH:O	2.62	0.47
3:F:37:ASP:O	3:F:38:ALA:C	2.47	0.47
3:F:22:ALA:O	3:F:23:VAL:C	2.53	0.47
3:C:55:TYR:HA	3:C:83:ILE:CG1	2.38	0.47
3:C:37:ASP:O	3:C:38:ALA:C	2.51	0.47
3:F:53:ARG:CG	3:F:67:GLY:HA3	2.45	0.46
3:F:23:VAL:HG22	4:F:140:HOH:O	2.15	0.46
2:B:212:DT:H2''	2:B:213:DG:H8	1.81	0.46
3:C:108:LEU:HA	3:C:108:LEU:HD23	1.44	0.46
3:F:63:LEU:HD22	3:F:83:ILE:HD11	1.97	0.46
3:F:2:PRO:HD3	3:F:105:PRO:CD	2.45	0.46
3:F:3:LEU:H	3:F:3:LEU:CD2	2.29	0.46
3:F:10:LEU:O	3:F:16:TYR:HB2	2.16	0.46
3:C:92:CYS:O	3:C:95:ILE:N	2.47	0.46
3:C:3:LEU:HD12	3:C:36:LEU:HB3	1.97	0.46
3:C:54:VAL:HG13	4:C:124:HOH:O	2.16	0.46
2:E:214:DG:OP1	3:F:53:ARG:HB2	2.16	0.46
2:E:220:DT:H72	4:E:121:HOH:O	2.15	0.46
3:C:108:LEU:O	3:C:111:LYS:N	2.49	0.45
3:F:97:HIS:ND1	4:F:120:HOH:O	2.21	0.45
3:F:107:GLU:HG2	3:F:111:LYS:HZ3	1.81	0.45
1:D:203:DG:H3'	3:F:23:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:LYS:HB2	3:C:84:THR:HB	1.98	0.45
3:C:4:GLY:HA2	3:C:104:PHE:HE2	1.81	0.45
2:E:218:DC:H2''	2:E:219:DT:O5'	2.16	0.45
4:A:94:HOH:O	2:B:219:DT:H72	2.17	0.45
3:F:10:LEU:O	3:F:16:TYR:CB	2.65	0.45
3:C:78:THR:CA	4:C:144:HOH:O	2.61	0.45
3:F:80:TYR:HD1	3:F:80:TYR:N	2.14	0.44
3:F:53:ARG:CZ	3:F:70:THR:HG22	2.47	0.44
2:B:214:DG:OP1	3:C:50:GLY:HA3	2.17	0.44
2:E:217:DC:C2	2:E:218:DC:C4	3.05	0.44
3:C:53:ARG:NE	3:C:70:THR:HG22	2.32	0.44
3:C:62:THR:HG22	3:C:62:THR:O	2.17	0.44
3:F:33:LEU:O	3:F:34:TYR:C	2.54	0.44
1:D:205:DA:H2'	1:D:206:DT:C6	2.52	0.44
3:F:92:CYS:HB3	4:F:127:HOH:O	2.18	0.44
3:F:27:MET:HB3	3:F:27:MET:CE	2.47	0.44
3:C:46:GLU:H	3:C:46:GLU:HG3	1.54	0.43
3:F:63:LEU:HD13	3:F:83:ILE:CD1	2.48	0.43
3:F:65:LYS:HE3	4:F:133:HOH:O	2.18	0.43
3:C:30:LEU:HA	3:C:30:LEU:HD23	1.73	0.43
3:C:78:THR:HB	3:C:79:PRO:HD2	1.99	0.43
3:C:96:GLU:HB3	4:C:169:HOH:O	2.19	0.43
3:F:92:CYS:SG	3:F:113:CYS:HB2	2.59	0.43
3:F:74:HIS:HA	3:F:81:TRP:CZ3	2.53	0.43
3:F:95:ILE:HG23	3:F:95:ILE:HD12	1.78	0.43
1:D:204:DG:P	3:F:22:ALA:HB3	2.59	0.43
3:F:70:THR:HB	3:F:83:ILE:HG23	2.00	0.42
3:C:74:HIS:HE1	4:C:141:HOH:O	1.94	0.42
3:C:75:VAL:HG12	3:C:78:THR:O	2.19	0.42
3:F:37:ASP:HB3	3:F:40:ALA:HB3	2.01	0.42
2:B:211:DT:C7	4:D:69:HOH:O	2.63	0.42
2:E:215:DA:C2'	2:E:216:DT:H72	2.38	0.42
3:F:90:ARG:O	3:F:94:MET:HG3	2.20	0.42
1:A:201:DA:H2'	4:A:43:HOH:O	2.19	0.42
3:C:19:GLN:H	3:C:19:GLN:HG2	1.20	0.42
3:F:3:LEU:H	3:F:3:LEU:HD23	1.85	0.42
1:A:201:DA:N6	2:B:219:DT:O4	2.52	0.42
3:F:5:SER:O	3:F:8:ARG:HB2	2.20	0.42
3:C:84:THR:O	3:C:86:THR:N	2.52	0.42
3:C:95:ILE:HD12	3:C:95:ILE:HG23	1.76	0.41
3:C:66:ASN:CB	4:C:125:HOH:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:96:GLU:HG2	3:C:100:GLN:HE21	1.84	0.41
3:C:26:PHE:CZ	3:C:30:LEU:HD11	2.55	0.41
1:D:205:DA:H2''	1:D:206:DT:O4'	2.20	0.41
3:F:48:LEU:HD21	3:F:94:MET:HB3	2.02	0.41
3:C:91:LYS:HE3	3:C:91:LYS:HB2	1.81	0.41
3:F:25:ARG:HG3	3:F:25:ARG:NH1	2.34	0.41
3:C:93:SER:HA	3:C:96:GLU:HB2	2.02	0.41
2:B:212:DT:H73	4:B:31:HOH:O	2.20	0.41
3:C:18:GLU:O	3:C:20:LYS:HD2	2.21	0.41
3:C:27:MET:O	3:C:31:SER:HB2	2.21	0.41
3:F:36:LEU:HA	3:F:36:LEU:HD23	1.75	0.41
3:C:79:PRO:HG2	3:C:80:TYR:CD1	2.55	0.40
3:F:54:VAL:O	3:F:63:LEU:HD22	2.21	0.40
3:F:99:MET:CE	3:F:109:ILE:HD13	2.47	0.40
3:C:90:ARG:HG2	3:C:94:MET:HE2	2.03	0.40
3:F:51:ARG:HB2	3:F:51:ARG:HH11	1.82	0.40
2:B:218:DC:O5'	2:B:218:DC:H2'	2.21	0.40
1:A:210:DA:H1'	2:E:211:DT:O5'	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:DA:N3	1:D:201:DA:N3[10_665]	1.03	1.17
1:D:201:DA:N3	1:D:201:DA:C4[10_665]	2.05	0.15
1:D:201:DA:C2	1:D:201:DA:N3[10_665]	2.08	0.12
1:D:201:DA:C1'	1:D:201:DA:N9[10_665]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	
3	C	113/116 (97%)	89 (79%)	17 (15%)	7 (6%)	2	10
3	F	113/116 (97%)	89 (79%)	14 (12%)	10 (9%)	1	4
All	All	226/232 (97%)	178 (79%)	31 (14%)	17 (8%)	1	6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	74	HIS
3	F	78	THR
3	C	67	GLY
3	F	65	LYS
3	C	13	SER
3	C	72	PRO
3	F	79	PRO
3	C	76	PRO
3	C	77	GLY
3	C	78	THR
3	F	67	GLY
3	F	72	PRO
3	F	76	PRO
3	F	77	GLY
3	F	23	VAL
3	C	79	PRO
3	F	109	ILE

5.3.2 Protein sidechains ⓘ

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	
3	C	99/99 (100%)	77 (78%)	22 (22%)	1	5
3	F	99/99 (100%)	72 (73%)	27 (27%)	0	2
All	All	198/198 (100%)	149 (75%)	49 (25%)	1	3

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	5	SER
3	C	10	LEU
3	C	11	LEU
3	C	14	ASP
3	C	18	GLU
3	C	19	GLN
3	C	20	LYS
3	C	28	LEU
3	C	31	SER
3	C	39	GLN
3	C	45	THR
3	C	47	SER
3	C	52	THR
3	C	73	LYS
3	C	74	HIS
3	C	75	VAL
3	C	76	PRO
3	C	79	PRO
3	C	82	VAL
3	C	92	CYS
3	C	108	LEU
3	C	113	CYS
3	F	3	LEU
3	F	14	ASP
3	F	18	GLU
3	F	28	LEU
3	F	31	SER
3	F	35	SER
3	F	39	GLN
3	F	45	THR
3	F	51	ARG
3	F	64	LEU
3	F	66	ASN
3	F	68	ASN
3	F	69	GLN
3	F	72	PRO
3	F	74	HIS
3	F	75	VAL
3	F	76	PRO
3	F	79	PRO
3	F	82	VAL
3	F	83	ILE
3	F	85	ASN

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Mol	Chain	Res	Type
3	F	90	ARG
3	F	93	SER
3	F	99	MET
3	F	101	SER
3	F	113	CYS
3	F	115	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	24	ASN
3	C	74	HIS
3	C	100	GLN
3	F	68	ASN
3	F	69	GLN
3	F	100	GLN

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 ⓘ

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(Å ²)	Q<0.9
1	A	10/10 (100%)	-0.54	0 100 100	59, 86, 100, 102	0
1	D	10/10 (100%)	-0.35	0 100 100	73, 96, 105, 130	0
2	B	10/10 (100%)	-0.19	0 100 100	62, 80, 120, 131	0
2	E	10/10 (100%)	0.08	1 (10%) 9 4	80, 89, 140, 157	0
3	C	115/116 (99%)	-0.37	1 (0%) 85 64	33, 55, 79, 93	0
3	F	115/116 (99%)	-0.16	1 (0%) 85 64	70, 91, 106, 116	0
All	All	270/272 (99%)	-0.26	3 (1%) 82 58	33, 78, 105, 157	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	220	DT	4.2
3	C	74	HIS	2.5
3	F	74	HIS	2.5

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

There are no such residues in this entry.