



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:46 PM GMT

PDB ID : 4Z1X
Title : Crystal structure of LAGLIDADG homing endonuclease I-GzeII in complex with DNA target
Authors : Stoddard, B.L.; Lambert, A.R.; Kulshina, N.
Deposited on : 2015-03-27
Resolution : 2.80 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

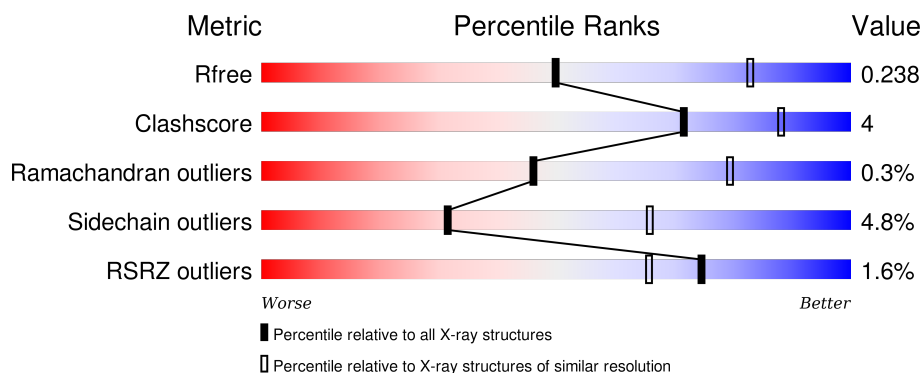
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	C	27	 4% 78% 22%
1	E	27	 70% 26% .
2	D	27	 4% 70% 22% . .
2	F	27	 81% 15% .
3	A	299	 2% 86% 10% . .

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Mol	Chain	Length	Quality of chain
3	B	299	<div><div><div>%</div><div><div></div></div><div>85%</div><div>11%</div><div></div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6906 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 DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	27	Total	C	N	O	P	0	0	0
			565	267	111	160	27			
1	E	27	Total	C	N	O	P	0	0	0
			562	267	111	158	26			

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	26	Total	C	N	O	P	0	0	0
			523	251	88	158	26			
2	F	26	Total	C	N	O	P	0	0	0
			520	251	88	156	25			

- Molecule 3 is a protein called LAGLIDADG endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	291	Total	C	N	O	S	0	0	0
			2301	1480	392	420	9			
3	B	291	Total	C	N	O	S	0	0	0
			2302	1487	394	412	9			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	-	expression tag	UNP A5J036
A	3	LEU	-	expression tag	UNP A5J036
A	4	SER	-	expression tag	UNP A5J036
A	5	THR	-	expression tag	UNP A5J036
A	6	SER	-	expression tag	UNP A5J036
A	48	LYS	LEU	engineered mutation	UNP A5J036
A	56	ASN	ILE	engineered mutation	UNP A5J036
A	106	LYS	LEU	engineered mutation	UNP A5J036

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Chain	Residue	Modelled	Actual	Comment	Reference
A	154	SER	VAL	engineered mutation	UNP A5J036
A	155	ASN	ILE	engineered mutation	UNP A5J036
A	163	ASN	VAL	engineered mutation	UNP A5J036
A	265	LYS	LEU	engineered mutation	UNP A5J036
B	2	ASP	-	expression tag	UNP A5J036
B	3	LEU	-	expression tag	UNP A5J036
B	4	SER	-	expression tag	UNP A5J036
B	5	THR	-	expression tag	UNP A5J036
B	6	SER	-	expression tag	UNP A5J036
B	48	LYS	LEU	engineered mutation	UNP A5J036
B	56	ASN	ILE	engineered mutation	UNP A5J036
B	106	LYS	LEU	engineered mutation	UNP A5J036
B	154	SER	VAL	engineered mutation	UNP A5J036
B	155	ASN	ILE	engineered mutation	UNP A5J036
B	163	ASN	VAL	engineered mutation	UNP A5J036
B	265	LYS	LEU	engineered mutation	UNP A5J036

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Ca 2 2	0	0
4	A	2	Total Ca 2 2	0	0

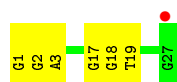
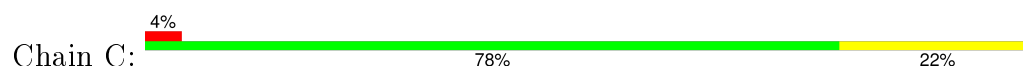
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	12	Total O 12 12	0	0
5	D	24	Total O 24 24	0	0
5	E	16	Total O 16 16	0	0
5	F	20	Total O 20 20	0	0
5	A	32	Total O 32 32	0	0
5	B	25	Total O 25 25	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: DNA (27-MER)



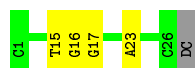
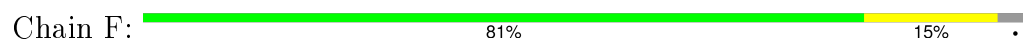
- Molecule 1: DNA (27-MER)



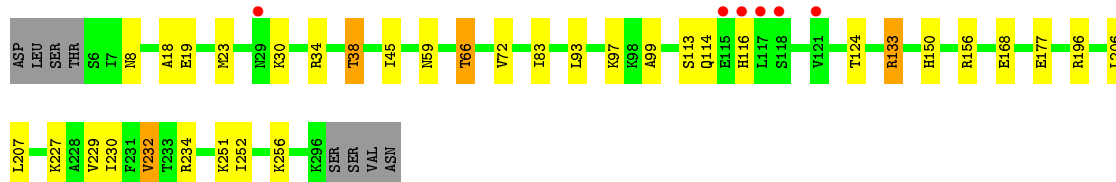
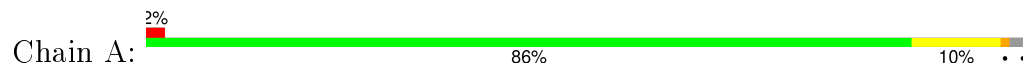
- Molecule 2: DNA (27-MER)



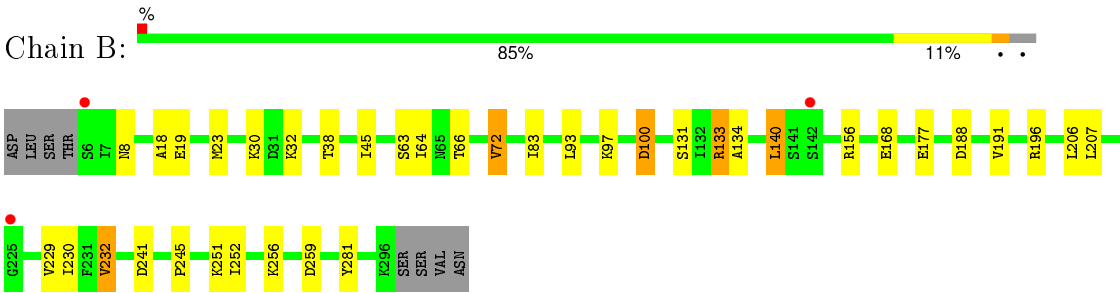
- Molecule 2: DNA (27-MER)



- Molecule 3: LAGLIDADG endonuclease



- Molecule 3: LAGLIDADG endonuclease



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.83 Å 61.19 Å 128.87 Å 90.00° 116.30° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 41.50 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.80) 98.7 (41.50-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.81 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.240 0.177 , 0.238	Depositor DCC
R_{free} test set	1111 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.4	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 21777 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6906	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0928e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

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

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	C	0.53	0/636	0.99	3/982 (0.3%)
1	E	0.56	1/633 (0.2%)	0.96	2/978 (0.2%)
2	D	0.55	1/583 (0.2%)	0.89	0/895
2	F	0.52	0/580	0.90	0/891
3	A	0.64	0/2354	0.75	4/3178 (0.1%)
3	B	0.63	0/2356	0.77	3/3180 (0.1%)
All	All	0.60	2/7142 (0.0%)	0.83	12/10104 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	15	DT	O3'-P	-6.61	1.53	1.61
1	E	16	DT	O3'-P	5.22	1.67	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	DG	O5'-P-OP1	7.45	119.64	110.70
1	C	17	DG	C1'-O4'-C4'	-6.92	103.18	110.10
3	A	234	ARG	CG-CD-NE	-6.81	97.51	111.80
1	E	17	DG	C1'-O4'-C4'	-6.29	103.81	110.10
1	C	19	DT	O5'-P-OP2	-6.03	100.27	105.70
3	A	133	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	16	DT	O5'-P-OP2	-5.96	100.34	105.70
3	A	133	ARG	NE-CZ-NH1	5.65	123.12	120.30
3	B	133	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	B	133	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	B	232	VAL	CB-CA-C	-5.34	101.25	111.40
3	A	232	VAL	CB-CA-C	-5.21	101.49	111.40

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	C	565	0	304	2	0
1	E	562	0	305	7	0
2	D	523	0	295	11	1
2	F	520	0	296	6	0
3	A	2301	0	2234	18	1
3	B	2302	0	2253	19	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	32	0	0	6	0
5	B	25	0	0	1	0
5	C	12	0	0	0	0
5	D	24	0	0	4	0
5	E	16	0	0	1	0
5	F	20	0	0	1	0
All	All	6906	0	5687	54	1

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 (54) 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:23:DA:H2'	5:F:112:HOH:O	1.71	0.89
2:D:16:DG:OP2	5:D:101:HOH:O	1.94	0.84
2:F:17:DG:H3'	3:A:23:MET:HE3	1.66	0.78
1:E:16:DT:O3'	5:E:101:HOH:O	2.04	0.75
2:D:23:DA:H2''	2:D:24:DT:OP2	1.90	0.70
3:B:134:ALA:HA	3:B:140:LEU:HD13	1.74	0.70
3:A:38:THR:HG22	5:A:502:HOH:O	1.91	0.69
2:D:16:DG:OP1	5:D:102:HOH:O	2.12	0.68
3:A:19:GLU:OE1	5:A:501:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:DG:OP2	3:B:19:GLU:OE1	2.14	0.65
2:D:17:DG:H3'	3:B:23:MET:HE3	1.78	0.65
5:D:101:HOH:O	3:B:177:GLU:OE1	2.15	0.63
2:D:16:DG:P	5:D:102:HOH:O	2.56	0.62
2:D:15:DT:H2''	2:D:16:DG:H5''	1.82	0.62
2:F:17:DG:H3'	3:A:23:MET:CE	2.28	0.62
2:D:17:DG:H3'	3:B:23:MET:CE	2.30	0.62
3:A:207:LEU:HD12	3:A:229:VAL:HG23	1.82	0.61
3:B:207:LEU:HD12	3:B:229:VAL:HG23	1.84	0.59
1:E:3:DA:H2''	1:E:4:DT:OP2	2.03	0.57
2:F:15:DT:H2''	2:F:16:DG:H5''	1.87	0.57
2:D:15:DT:C2'	2:D:16:DG:H5''	2.34	0.56
1:E:5:DG:N7	3:A:34:ARG:NH2	2.45	0.54
1:C:3:DA:OP1	3:B:32:LYS:NZ	2.41	0.53
2:F:15:DT:C2'	2:F:16:DG:H5''	2.40	0.52
1:E:3:DA:C2'	1:E:4:DT:OP2	2.59	0.51
3:A:8:ASN:CG	3:A:168:GLU:HG2	2.33	0.50
3:B:8:ASN:CG	3:B:168:GLU:HG2	2.32	0.49
3:B:196:ARG:HG2	3:B:232:VAL:HG13	1.97	0.47
3:A:196:ARG:HG2	3:A:232:VAL:HG13	1.96	0.47
3:A:116:HIS:CD2	5:A:513:HOH:O	2.67	0.47
2:F:17:DG:C3'	3:A:23:MET:HE3	2.40	0.47
3:A:177:GLU:OE1	5:A:501:HOH:O	2.21	0.46
3:A:113:SER:O	3:A:114:GLN:HB2	2.16	0.46
3:B:18:ALA:HB1	3:B:177:GLU:HG2	1.97	0.46
1:E:19:DT:H2''	1:E:20:DA:O5'	2.16	0.45
3:B:45:ILE:HD13	3:B:66:THR:HG23	1.99	0.44
1:E:16:DT:P	5:A:501:HOH:O	2.77	0.43
3:A:18:ALA:HB1	3:A:177:GLU:HG2	2.01	0.43
1:E:18:DG:H2''	1:E:19:DT:O5'	2.19	0.43
3:A:59:ASN:HA	5:A:523:HOH:O	2.18	0.43
3:A:252:ILE:HD11	3:A:256:LYS:C	2.39	0.43
3:B:100:ASP:OD1	3:B:156:ARG:NH2	2.52	0.42
2:D:17:DG:C3'	3:B:23:MET:HE3	2.48	0.42
3:B:252:ILE:HD11	3:B:256:LYS:C	2.40	0.42
3:A:230:ILE:HD12	3:A:232:VAL:HG22	2.01	0.42
3:B:64:ILE:HA	3:B:72:VAL:O	2.19	0.41
2:D:17:DG:H2''	2:D:18:DT:H5'	2.02	0.41
3:B:241:ASP:O	3:B:245:PRO:HG2	2.20	0.41
3:B:230:ILE:HD12	3:B:232:VAL:HG22	2.01	0.41
3:B:259:ASP:OD2	5:B:501:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:45:ILE:HD13	3:A:66:THR:HG22	2.03	0.41
3:B:191:VAL:HG23	3:B:281:TYR:CE2	2.56	0.40
1:C:1:DG:C2'	1:C:2:DG:H5'	2.52	0.40
3:A:99:ALA:HB3	3:A:156:ARG:NH1	2.36	0.40

All (1) 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)
2:D:3:DT:OP1	3:A:150:HIS:NE2[2_464]	2.13	0.07

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	A	289/299 (97%)	273 (94%)	15 (5%)	1 (0%)	46	79
3	B	289/299 (97%)	275 (95%)	13 (4%)	1 (0%)	46	79
All	All	578/598 (97%)	548 (95%)	28 (5%)	2 (0%)	46	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	30	LYS
3	B	30	LYS

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	A	248/278 (89%)	237 (96%)	11 (4%)	35	69
3	B	247/278 (89%)	234 (95%)	13 (5%)	28	61
All	All	495/556 (89%)	471 (95%)	24 (5%)	31	66

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	38	THR
3	A	66	THR
3	A	72	VAL
3	A	83	ILE
3	A	93	LEU
3	A	97	LYS
3	A	124	THR
3	A	133	ARG
3	A	206	LEU
3	A	227	LYS
3	A	251	LYS
3	B	38	THR
3	B	63	SER
3	B	72	VAL
3	B	83	ILE
3	B	93	LEU
3	B	97	LYS
3	B	100	ASP
3	B	131	SER
3	B	133	ARG
3	B	140	LEU
3	B	188	ASP
3	B	206	LEU
3	B	251	LYS

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

Mol	Chain	Res	Type
3	B	199	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](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	27/27 (100%)	-0.06	1 (3%) 45 33	28, 47, 87, 150	0
1	E	27/27 (100%)	-0.06	0 100 100	28, 54, 70, 81	0
2	D	26/27 (96%)	-0.39	1 (3%) 44 32	29, 46, 78, 98	0
2	F	26/27 (96%)	-0.18	0 100 100	22, 48, 75, 87	0
3	A	291/299 (97%)	-0.37	6 (2%) 67 56	16, 35, 66, 103	0
3	B	291/299 (97%)	-0.40	3 (1%) 84 77	21, 39, 67, 86	0
All	All	688/706 (97%)	-0.35	11 (1%) 74 66	16, 39, 71, 150	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	29	ASN	4.0
3	A	118	SER	3.2
3	B	142	SER	3.1
3	A	117	LEU	2.9
3	A	116	HIS	2.7
3	B	6	SER	2.6
3	A	121	VAL	2.3
1	C	27	DG	2.2
3	B	225	GLY	2.1
3	A	115	GLU	2.1
2	D	1	DC	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 [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	A	401	1/1	0.98	0.14	-0.62	21,21,21,21	0
4	CA	B	401	1/1	0.91	0.11	-1.22	30,30,30,30	0
4	CA	B	402	1/1	0.97	0.11	-1.79	32,32,32,32	0
4	CA	A	402	1/1	0.98	0.07	-4.31	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.