



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 05:57 AM UTC

PDB ID : 1U8R / pdb_00001u8r
Title : Crystal Structure of an IdeR-DNA Complex Reveals a Conformational Change
in Activated IdeR for Base-specific Interactions
Authors : Wisedchaisri, G.; Holmes, R.K.; Hol, W.G.J.
Deposited on : 2004-08-06
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

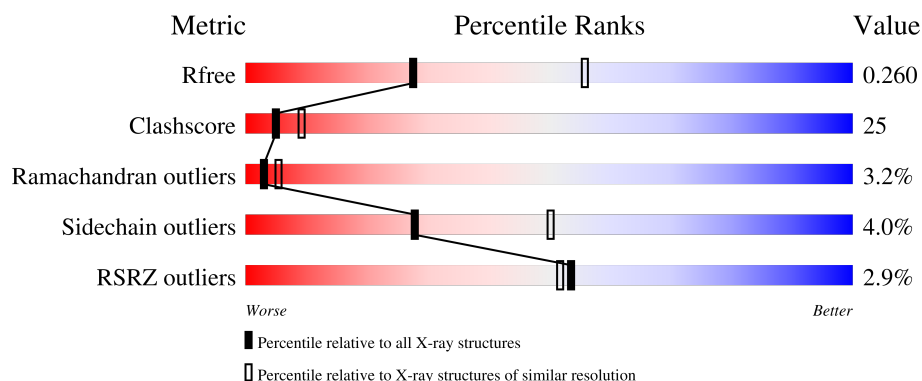
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

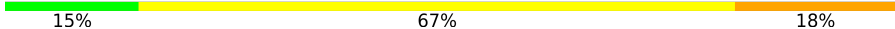
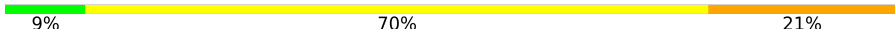
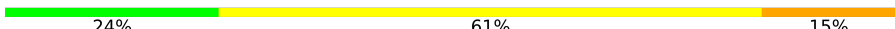
The reported resolution of this entry is 2.75 Å.

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 $\leq 5\%$. 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	E	33	
1	K	33	
2	F	33	
2	L	33	
3	A	230	

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Mol	Chain	Length	Quality of chain
3	B	230	3%53%37%5% . .
3	C	230	2%54%38%. .
3	D	230	3%50%41%. . .
3	G	230	2%56%36%. .
3	H	230	3%52%40%. . .
3	I	230	7%53%39%. .
3	J	230	2%56%37%. . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16481 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 mbtA operator DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	33	Total	C	N	O	P	0	0	0
			670	321	117	200	32			
1	K	33	Total	C	N	O	P	0	0	0
			670	321	117	200	32			

- Molecule 2 is a DNA chain called mbtB operator DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	33	Total	C	N	O	P	0	0	0
			677	322	131	192	32			
2	L	33	Total	C	N	O	P	0	0	0
			677	322	131	192	32			

- Molecule 3 is a protein called Iron-dependent repressor ideR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	B	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	C	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	D	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	G	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	H	222	Total	C	N	O	S	0	0	0
			1719	1071	314	327	7			
3	I	221	Total	C	N	O	S	0	0	0
			1711	1067	312	325	7			
3	J	222	Total	C	N	O	S	0	0	0
			1719	1071	314	327	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	136	ASP	VAL	SEE REMARK 999	UNP P0A672
B	136	ASP	VAL	SEE REMARK 999	UNP P0A672
C	136	ASP	VAL	SEE REMARK 999	UNP P0A672
D	136	ASP	VAL	SEE REMARK 999	UNP P0A672
G	136	ASP	VAL	SEE REMARK 999	UNP P0A672
H	136	ASP	VAL	SEE REMARK 999	UNP P0A672
I	136	ASP	VAL	SEE REMARK 999	UNP P0A672
J	136	ASP	VAL	SEE REMARK 999	UNP P0A672

- Molecule 4 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Co 3 3	0	0
4	B	3	Total Co 3 3	0	0
4	C	3	Total Co 3 3	0	0
4	D	3	Total Co 3 3	0	0
4	G	3	Total Co 3 3	0	0
4	H	3	Total Co 3 3	0	0
4	I	3	Total Co 3 3	0	0
4	J	3	Total Co 3 3	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	G	1	Total Na 1 1	0	0

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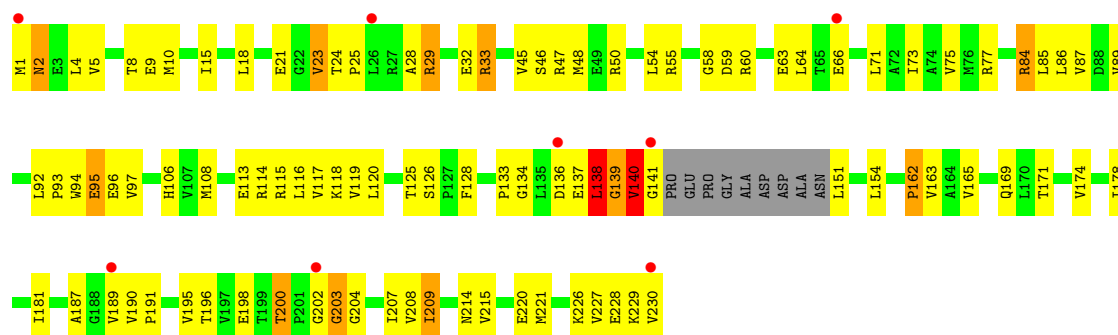
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total 1	Na 1	0	0
5	I	1	Total 1	Na 1	0	0
5	J	1	Total 1	Na 1	0	0

- Molecule 6 is water.

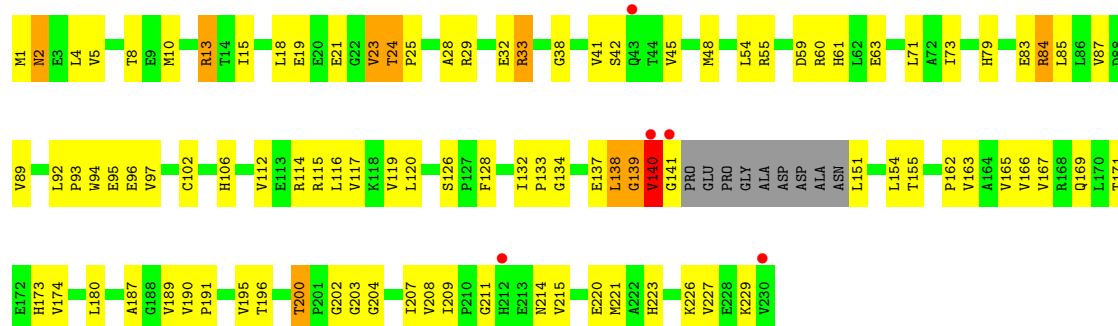
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total 1	O 1	0	0
6	F	7	Total 7	O 7	0	0
6	K	2	Total 2	O 2	0	0
6	L	9	Total 9	O 9	0	0
6	A	2	Total 2	O 2	0	0
6	B	3	Total 3	O 3	0	0
6	C	6	Total 6	O 6	0	0
6	D	7	Total 7	O 7	0	0
6	G	3	Total 3	O 3	0	0
6	H	5	Total 5	O 5	0	0
6	I	4	Total 4	O 4	0	0
6	J	2	Total 2	O 2	0	0



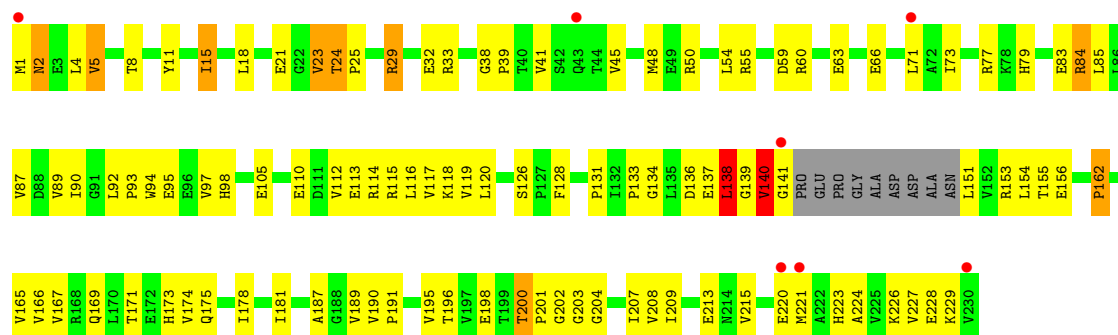
• Molecule 3: Iron-dependent repressor ideR



• Molecule 3: Iron-dependent repressor ideR

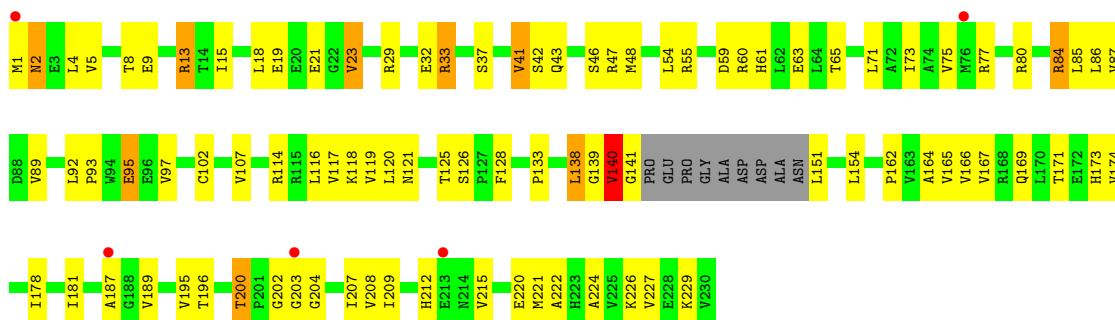


• Molecule 3: Iron-dependent repressor ideR

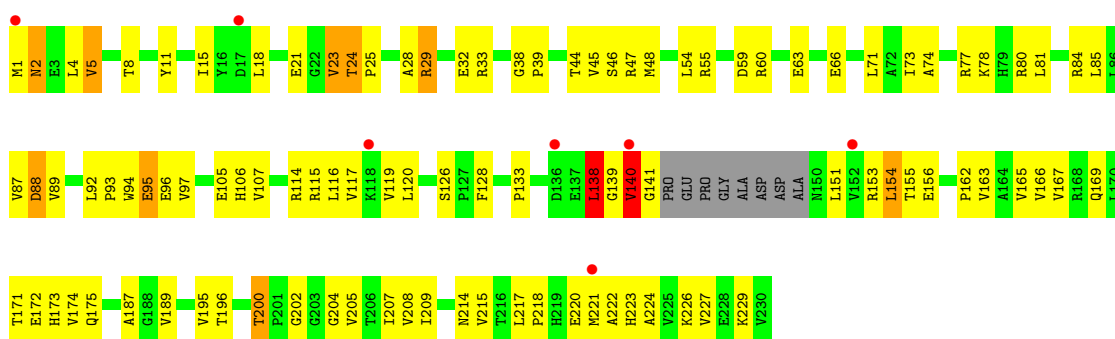


• Molecule 3: Iron-dependent repressor ideR

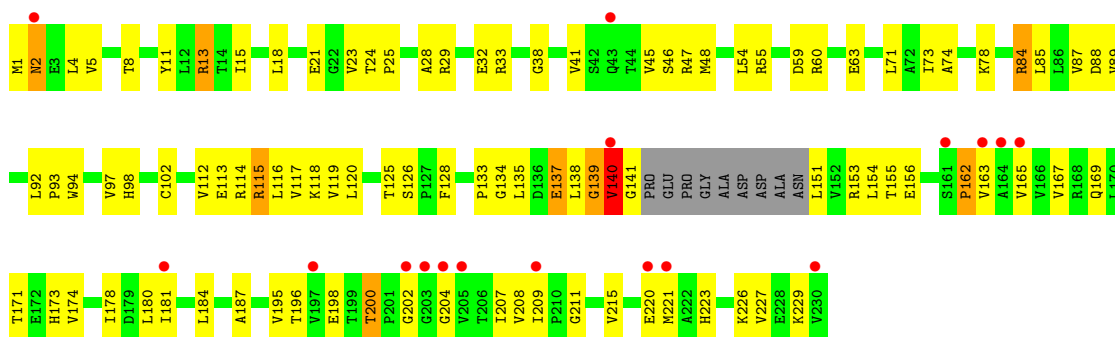




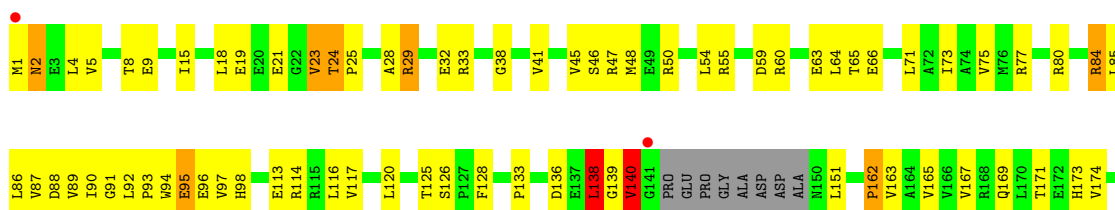
• Molecule 3: Iron-dependent repressor ideR

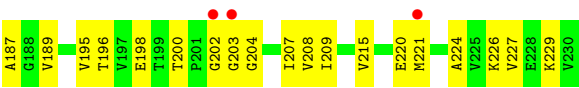


• Molecule 3: Iron-dependent repressor ideR



• Molecule 3: Iron-dependent repressor ideR





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	107.96Å 107.96Å 215.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.75 – 2.75 46.75 – 2.75	Depositor EDS
% Data completeness (in resolution range)	86.6 (46.75-2.75) 86.7 (46.75-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.81	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.265 0.231 , 0.260	Depositor DCC
R_{free} test set	3193 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.886	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for -h,-k,l 0.106 for h,-h-k,-l 0.049 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16481	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: NA, CO

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	E	0.40	0/749	0.85	0/1154
1	K	0.38	0/749	0.86	1/1154 (0.1%)
2	F	0.39	0/761	0.92	2/1173 (0.2%)
2	L	0.37	0/761	0.90	4/1173 (0.3%)
3	A	0.54	0/1737	0.98	7/2361 (0.3%)
3	B	0.48	0/1737	0.95	2/2361 (0.1%)
3	C	0.49	0/1737	0.96	5/2361 (0.2%)
3	D	0.51	0/1737	0.97	5/2361 (0.2%)
3	G	0.52	0/1737	0.94	2/2361 (0.1%)
3	H	0.49	0/1745	0.98	6/2372 (0.3%)
3	I	0.49	0/1737	0.96	2/2361 (0.1%)
3	J	0.50	0/1745	0.97	5/2372 (0.2%)
All	All	0.48	0/16932	0.95	41/23564 (0.2%)

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	E	0	6
1	K	0	6
2	F	0	5
2	L	0	3
All	All	0	20

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	33	ARG	N-CA-C	7.17	119.10	111.28
3	I	33	ARG	N-CA-C	6.46	118.33	111.28
2	L	19	DC	N1-C1'-C2'	-6.30	104.05	113.50
3	G	33	ARG	N-CA-C	6.05	118.67	111.71
3	B	33	ARG	N-CA-C	6.04	118.65	111.71

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	10	DC	Sidechain
1	E	15	DG	Sidechain
1	E	16	DC	Sidechain
1	E	20	DC	Sidechain
1	E	5	DG	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	E	670	0	375	42	0
1	K	670	0	375	40	0
2	F	677	0	371	32	0
2	L	677	0	371	33	0
3	A	1711	0	1748	75	0
3	B	1711	0	1748	91	0
3	C	1711	0	1748	83	0
3	D	1711	0	1748	90	0
3	G	1711	0	1748	76	0
3	H	1719	0	1754	88	0
3	I	1711	0	1748	81	0
3	J	1719	0	1754	89	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	I	3	0	0	0	0
4	J	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	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
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	A	2	0	0	1	0
6	B	3	0	0	1	0
6	C	6	0	0	1	0
6	D	7	0	0	0	0
6	E	1	0	0	0	0
6	F	7	0	0	0	0
6	G	3	0	0	1	0
6	H	5	0	0	0	0
6	I	4	0	0	1	0
6	J	2	0	0	0	0
6	K	2	0	0	0	0
6	L	9	0	0	0	0
All	All	16481	0	15488	799	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 25.

The worst 5 of 799 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:H:84:ARG:HG3	3:H:120:LEU:HD13	1.33	1.06
1:E:28:DT:H2''	1:E:29:DA:H5''	1.39	1.05
1:K:28:DT:H2''	1:K:29:DA:H5''	1.36	1.03
3:B:174:VAL:HA	3:B:221:MET:HE1	1.43	1.01
2:F:2:DA:H2''	2:F:3:DC:H5'	1.45	0.98

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	
3	A	217/230 (94%)	186 (86%)	24 (11%)	7 (3%)	3	5
3	B	217/230 (94%)	186 (86%)	23 (11%)	8 (4%)	2	4
3	C	217/230 (94%)	192 (88%)	18 (8%)	7 (3%)	3	5
3	D	217/230 (94%)	190 (88%)	18 (8%)	9 (4%)	2	3
3	G	217/230 (94%)	189 (87%)	21 (10%)	7 (3%)	3	5
3	H	218/230 (95%)	190 (87%)	21 (10%)	7 (3%)	3	5
3	I	217/230 (94%)	191 (88%)	21 (10%)	5 (2%)	5	9
3	J	218/230 (95%)	193 (88%)	19 (9%)	6 (3%)	4	6
All	All	1738/1840 (94%)	1517 (87%)	165 (10%)	56 (3%)	3	5

5 of 56 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	140	VAL
3	B	140	VAL
3	C	140	VAL
3	D	140	VAL
3	G	140	VAL

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	
3	A	189/195 (97%)	179 (95%)	10 (5%)	20	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	189/195 (97%)	181 (96%)	8 (4%)	26	49
3	C	189/195 (97%)	182 (96%)	7 (4%)	30	54
3	D	189/195 (97%)	182 (96%)	7 (4%)	30	54
3	G	189/195 (97%)	181 (96%)	8 (4%)	26	49
3	H	190/195 (97%)	184 (97%)	6 (3%)	34	58
3	I	189/195 (97%)	181 (96%)	8 (4%)	26	49
3	J	190/195 (97%)	184 (97%)	6 (3%)	34	58
All	All	1514/1560 (97%)	1454 (96%)	60 (4%)	28	50

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	84	ARG
3	J	29	ARG
3	G	71	LEU
3	J	23	VAL
3	J	140	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	121	ASN
3	J	130	ASN
3	D	192	ASN
3	D	121	ASN
3	J	169	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 32 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 [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	E	33/33 (100%)	-0.13	0 100 100	46, 69, 122, 126	0
1	K	33/33 (100%)	-0.03	0 100 100	46, 75, 164, 173	0
2	F	33/33 (100%)	-0.15	0 100 100	43, 74, 106, 109	0
2	L	33/33 (100%)	0.08	0 100 100	50, 78, 151, 160	0
3	A	221/230 (96%)	0.15	2 (0%) 81 81	32, 73, 124, 170	3 (1%)
3	B	221/230 (96%)	0.35	8 (3%) 46 44	44, 82, 132, 152	3 (1%)
3	C	221/230 (96%)	0.30	5 (2%) 61 59	44, 83, 142, 199	3 (1%)
3	D	221/230 (96%)	0.13	7 (3%) 50 48	36, 74, 122, 166	3 (1%)
3	G	221/230 (96%)	0.19	5 (2%) 61 59	39, 73, 122, 171	3 (1%)
3	H	222/230 (96%)	0.36	7 (3%) 50 48	40, 82, 133, 176	3 (1%)
3	I	221/230 (96%)	0.43	17 (7%) 19 19	39, 85, 155, 200	3 (1%)
3	J	222/230 (96%)	0.17	5 (2%) 61 59	44, 74, 127, 146	3 (1%)
All	All	1902/1972 (96%)	0.24	56 (2%) 53 52	32, 79, 137, 200	24 (1%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	43	GLN	4.2
3	I	43	GLN	3.9
3	D	230	VAL	3.7
3	J	141	GLY	3.6
3	D	43	GLN	3.5

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
5	NA	D	4104	1/1	0.82	0.21	50,50,50,50	0
5	NA	J	8108	1/1	0.88	0.22	50,50,50,50	0
5	NA	C	3103	1/1	0.91	0.22	58,58,58,58	0
5	NA	A	1101	1/1	0.91	0.07	65,65,65,65	0
5	NA	B	2102	1/1	0.91	0.18	41,41,41,41	0
5	NA	H	6106	1/1	0.92	0.21	59,59,59,59	0
5	NA	G	5105	1/1	0.93	0.13	51,51,51,51	0
5	NA	I	7107	1/1	0.94	0.14	50,50,50,50	0
4	CO	I	7003	1/1	0.96	0.11	90,90,90,90	0
4	CO	A	1003	1/1	0.96	0.11	73,73,73,73	0
4	CO	B	2003	1/1	0.96	0.06	85,85,85,85	0
4	CO	H	6003	1/1	0.97	0.09	85,85,85,85	0
4	CO	J	8003	1/1	0.97	0.09	78,78,78,78	0
4	CO	C	3003	1/1	0.98	0.04	73,73,73,73	0
4	CO	I	7002	1/1	0.98	0.07	66,66,66,66	0
4	CO	D	4003	1/1	0.98	0.09	73,73,73,73	0
4	CO	I	7001	1/1	0.99	0.03	73,73,73,73	0
4	CO	A	1002	1/1	0.99	0.06	60,60,60,60	0
4	CO	C	3002	1/1	0.99	0.05	61,61,61,61	0
4	CO	J	8001	1/1	0.99	0.03	56,56,56,56	0
4	CO	J	8002	1/1	0.99	0.03	55,55,55,55	0
4	CO	A	1001	1/1	0.99	0.03	65,65,65,65	0
4	CO	D	4002	1/1	0.99	0.03	48,48,48,48	0
4	CO	B	2001	1/1	0.99	0.03	67,67,67,67	0
4	CO	G	5001	1/1	0.99	0.01	52,52,52,52	0
4	CO	G	5002	1/1	0.99	0.02	45,45,45,45	0
4	CO	G	5003	1/1	0.99	0.08	76,76,76,76	0
4	CO	H	6001	1/1	0.99	0.03	66,66,66,66	0
4	CO	H	6002	1/1	0.99	0.05	53,53,53,53	0
4	CO	B	2002	1/1	0.99	0.07	70,70,70,70	0
4	CO	C	3001	1/1	1.00	0.01	67,67,67,67	0
4	CO	D	4001	1/1	1.00	0.02	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.