



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:29 PM GMT

PDB ID : 1P4E
Title : Flpe W330F mutant-DNA Holliday Junction Complex
Authors : Rice, P.A.; Chen, Y.
Deposited on : 2003-04-23
Resolution : 2.70 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
<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

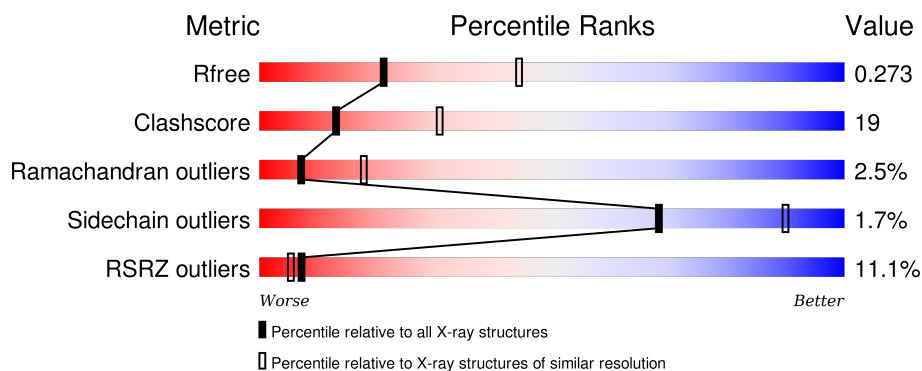
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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	E	13	<div> <div>15%</div> <div>85%</div> </div>
1	F	13	<div> <div>38%</div> <div>54%</div> <div>8%</div> </div>
2	I	20	<div> <div>10%</div> <div>35%</div> <div>65%</div> </div>
2	J	20	<div> <div>45%</div> <div>55%</div> </div>
3	G	33	<div> <div>30%</div> <div>70%</div> </div>

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Mol	Chain	Length	Quality of chain
3	H	33	
4	A	429	
4	B	429	
5	C	429	
5	D	429	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PTR	D	343	-	-	X	-
6	2PO	H	513	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16070 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(*TP*AP*AP*GP*TP*TP*CP*CP*TP*AP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	13	Total	C	N	O	P	0	0	0
			259	127	41	79	12			
1	F	13	Total	C	N	O	P	0	0	0
			259	127	41	79	12			

- Molecule 2 is a DNA chain called 5'-D(*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*TP*AP*GP*GP*AP*AP*CP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	20	Total	C	N	O	P	0	0	0
			395	189	75	112	19			
2	J	20	Total	C	N	O	P	0	0	0
			395	189	75	112	19			

- Molecule 3 is a DNA chain called 33-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	33	Total	C	N	O	P	0	0	0
			657	316	116	193	32			
3	H	33	Total	C	N	O	P	0	0	0
			654	316	116	191	31			

- Molecule 4 is a protein called Recombinase FLP protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	400	Total	C	N	O	S	0	0	0
			3242	2086	546	599	11			
4	B	413	Total	C	N	O	S	0	0	0
			3357	2157	573	616	11			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	PRO	SEE REMARK 999	UNP P03870
A	5	ASP	GLY	polymorphism	UNP P03870
A	33	SER	LEU	SEE REMARK 999	UNP P03870
A	108	ASN	TYR	SEE REMARK 999	UNP P03870
A	294	PRO	SER	SEE REMARK 999	UNP P03870
A	330	PHE	TRP	ENGINEERED	UNP P03870
A	424	GLY	-	EXPRESSION TAG	UNP P03870
A	425	HIS	-	EXPRESSION TAG	UNP P03870
A	426	HIS	-	EXPRESSION TAG	UNP P03870
A	427	HIS	-	EXPRESSION TAG	UNP P03870
A	428	HIS	-	EXPRESSION TAG	UNP P03870
A	429	HIS	-	EXPRESSION TAG	UNP P03870
A	430	HIS	-	EXPRESSION TAG	UNP P03870
B	2	SER	PRO	SEE REMARK 999	UNP P03870
B	5	ASP	GLY	polymorphism	UNP P03870
B	33	SER	LEU	SEE REMARK 999	UNP P03870
B	108	ASN	TYR	SEE REMARK 999	UNP P03870
B	294	PRO	SER	SEE REMARK 999	UNP P03870
B	330	PHE	TRP	ENGINEERED	UNP P03870
B	424	GLY	-	EXPRESSION TAG	UNP P03870
B	425	HIS	-	EXPRESSION TAG	UNP P03870
B	426	HIS	-	EXPRESSION TAG	UNP P03870
B	427	HIS	-	EXPRESSION TAG	UNP P03870
B	428	HIS	-	EXPRESSION TAG	UNP P03870
B	429	HIS	-	EXPRESSION TAG	UNP P03870
B	430	HIS	-	EXPRESSION TAG	UNP P03870

- Molecule 5 is a protein called Recombinase FLP protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	C	400	Total	C	N	O	P	S	0	0	0
			3263	2100	551	600	1	11			
5	D	409	Total	C	N	O	P	S	0	0	0
			3319	2132	562	613	1	11			

There are 26 discrepancies between the modelled and reference sequences:

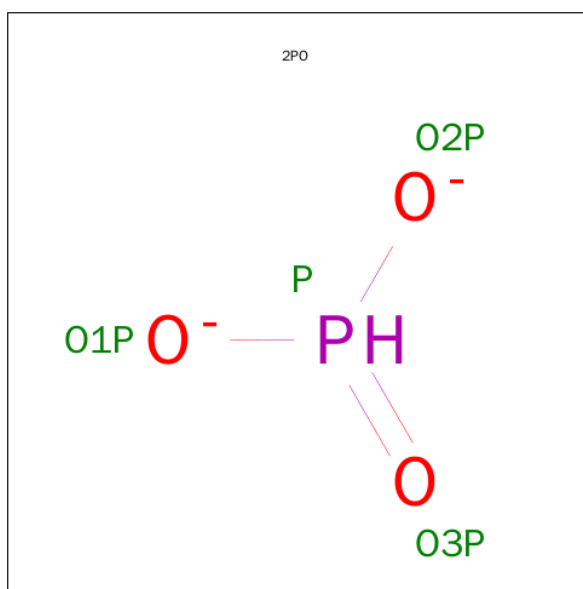
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	SER	PRO	SEE REMARK 999	UNP P03870
C	5	ASP	GLY	polymorphism	UNP P03870
C	33	SER	LEU	SEE REMARK 999	UNP P03870
C	108	ASN	TYR	SEE REMARK 999	UNP P03870
C	294	PRO	SER	SEE REMARK 999	UNP P03870

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Chain	Residue	Modelled	Actual	Comment	Reference
C	330	PHE	TRP	ENGINEERED	UNP P03870
C	424	GLY	-	EXPRESSION TAG	UNP P03870
C	425	HIS	-	EXPRESSION TAG	UNP P03870
C	426	HIS	-	EXPRESSION TAG	UNP P03870
C	427	HIS	-	EXPRESSION TAG	UNP P03870
C	428	HIS	-	EXPRESSION TAG	UNP P03870
C	429	HIS	-	EXPRESSION TAG	UNP P03870
C	430	HIS	-	EXPRESSION TAG	UNP P03870
D	2	SER	PRO	SEE REMARK 999	UNP P03870
D	5	ASP	GLY	polymorphism	UNP P03870
D	33	SER	LEU	SEE REMARK 999	UNP P03870
D	108	ASN	TYR	SEE REMARK 999	UNP P03870
D	294	PRO	SER	SEE REMARK 999	UNP P03870
D	330	PHE	TRP	ENGINEERED	UNP P03870
D	424	GLY	-	EXPRESSION TAG	UNP P03870
D	425	HIS	-	EXPRESSION TAG	UNP P03870
D	426	HIS	-	EXPRESSION TAG	UNP P03870
D	427	HIS	-	EXPRESSION TAG	UNP P03870
D	428	HIS	-	EXPRESSION TAG	UNP P03870
D	429	HIS	-	EXPRESSION TAG	UNP P03870
D	430	HIS	-	EXPRESSION TAG	UNP P03870

- Molecule 6 is PHOSPHONATE (three-letter code: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total O P 4 3 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	O 2	0	0
7	B	98	Total 98	O 98	0	0
7	C	24	Total 24	O 24	0	0
7	D	68	Total 68	O 68	0	0
7	F	13	Total 13	O 13	0	0
7	G	19	Total 19	O 19	0	0
7	H	14	Total 14	O 14	0	0
7	I	9	Total 9	O 9	0	0
7	J	19	Total 19	O 19	0	0

3 Residue-property plots

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(*TP*AP*AP*GP*TP*TP*CP*CP*TP*AP*TP*TP*C)-3'

Chain E: 



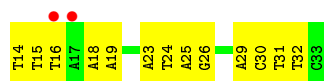
- Molecule 1: 5'-D(*TP*AP*AP*GP*TP*TP*CP*CP*TP*AP*TP*TP*C)-3'

Chain F: 



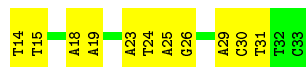
- Molecule 2: 5'-D(*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*TP*AP*GP*GP*AP*AP*CP*TP*TP*C)-3'

Chain I: 



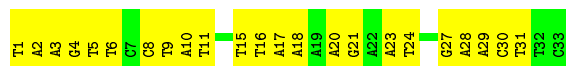
- Molecule 2: 5'-D(*TP*TP*TP*AP*AP*AP*AP*GP*AP*AP*TP*AP*GP*GP*AP*AP*CP*TP*TP*C)-3'

Chain J: 

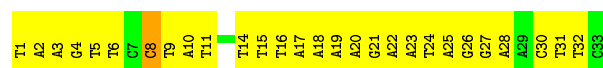


- Molecule 3: 33-MER

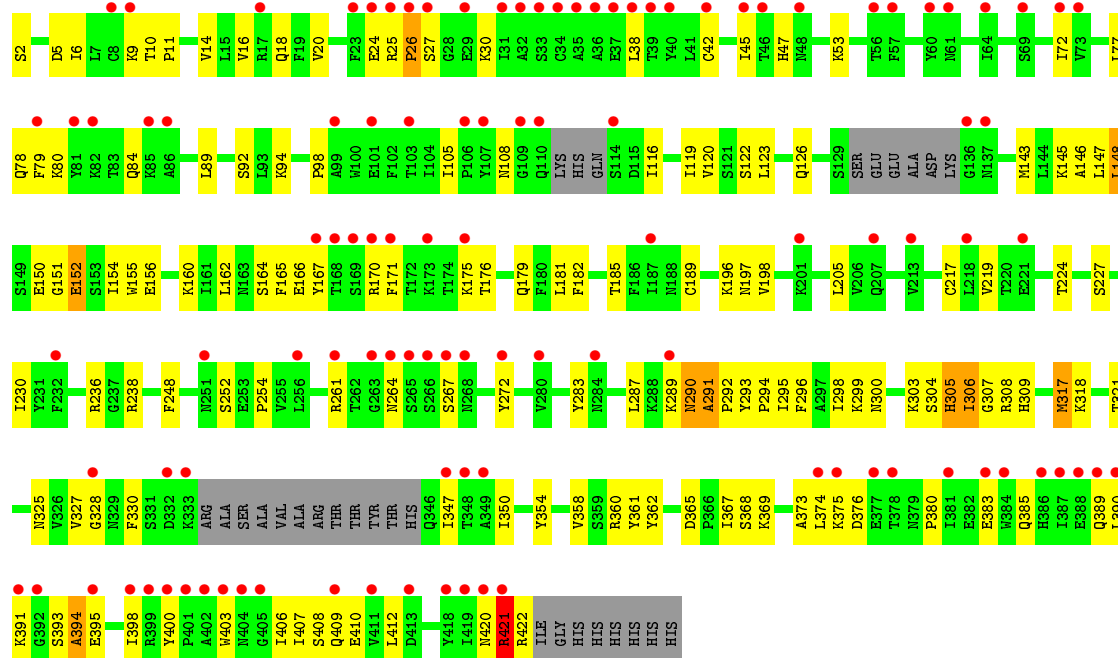
Chain G: 



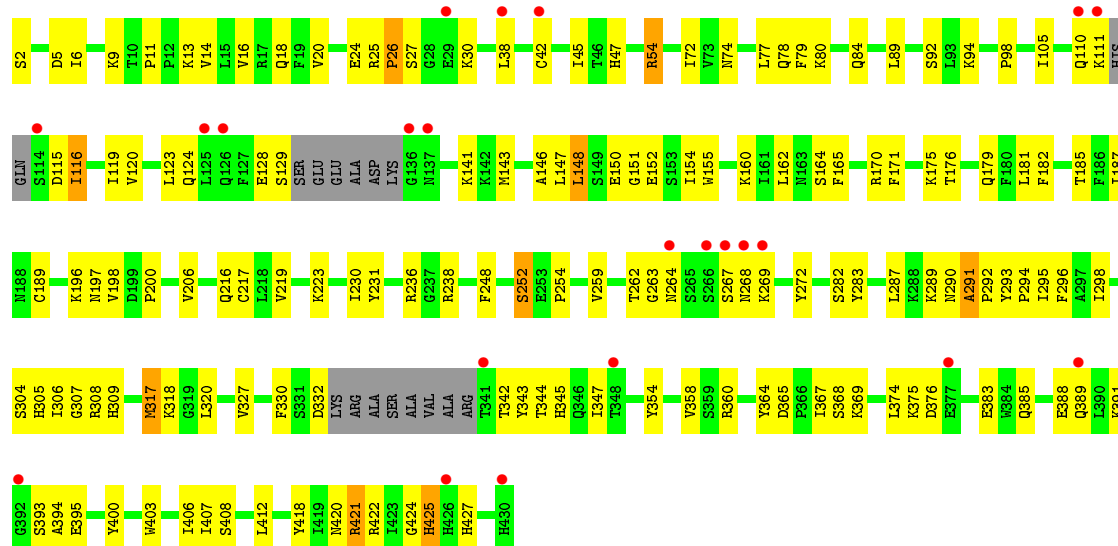
- Molecule 3: 33-MER



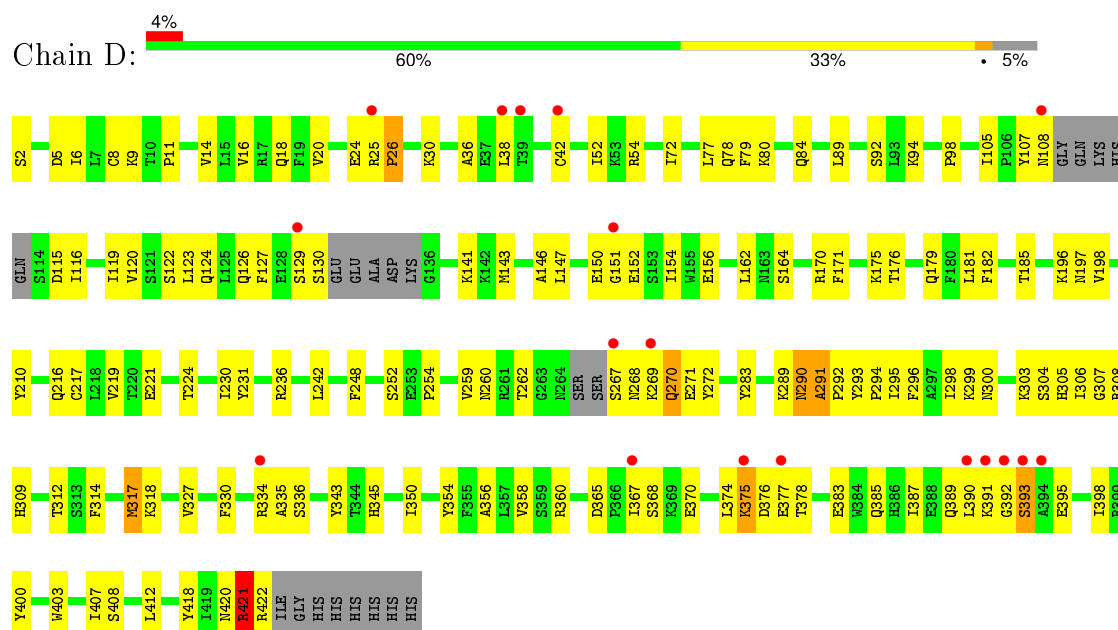
- Molecule 4: Recombinase FLP protein



- Molecule 4: Recombinase FLP protein



- Molecule 5: Recombinase FLP protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.76Å 116.72Å 142.05Å 90.00° 97.64° 90.00°	Depositor
Resolution (Å)	21.98 – 2.70 21.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.8 (21.98-2.70) 90.9 (21.98-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.275 0.235 , 0.273	Depositor DCC
R_{free} test set	6513 reflections (11.25%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 69141 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16070	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 3.84% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, 2PO

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	0.44	0/288	0.84	0/442
1	F	0.62	0/288	0.94	0/442
2	I	0.44	0/444	0.85	0/685
2	J	0.55	0/444	0.89	0/685
3	G	0.52	0/736	0.89	0/1135
3	H	0.50	0/732	0.88	0/1127
4	A	0.32	0/3311	0.55	0/4468
4	B	0.44	0/3434	0.62	0/4637
5	C	0.36	0/3316	0.59	1/4475 (0.0%)
5	D	0.41	0/3373	0.61	1/4552 (0.0%)
All	All	0.41	0/16366	0.66	2/22648 (0.0%)

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	F	0	1
3	H	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	270	GLN	N-CA-C	-5.44	96.32	111.00
5	D	270	GLN	N-CA-C	-5.38	96.47	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	8	DC	Sidechain
3	H	8	DC	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	259	0	150	22	0
1	F	259	0	150	9	0
2	I	395	0	216	22	0
2	J	395	0	216	20	0
3	G	657	0	365	27	0
3	H	654	0	366	56	0
4	A	3242	0	3278	122	0
4	B	3357	0	3371	130	0
5	C	3263	0	3295	101	0
5	D	3319	0	3352	123	0
6	H	4	0	0	2	0
7	A	2	0	0	0	0
7	B	98	0	0	10	0
7	C	24	0	0	3	0
7	D	68	0	0	6	0
7	F	13	0	0	0	0
7	G	19	0	0	0	0
7	H	14	0	0	2	0
7	I	9	0	0	1	0
7	J	19	0	0	0	0
All	All	16070	0	14759	580	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 19.

The worst 5 of 580 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:15:DT:H2"	3:H:16:DT:H5"	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:25:DA:H2''	2:I:26:DG:H5'	1.45	0.97
1:E:4:DG:H2''	1:E:5:DT:H5''	1.47	0.96
2:J:25:DA:H2''	2:J:26:DG:H5'	1.46	0.95
3:H:1:DT:H6	3:H:1:DT:H5'	1.32	0.95

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	
4	A	392/429 (91%)	345 (88%)	36 (9%)	11 (3%)	6	15
4	B	405/429 (94%)	363 (90%)	32 (8%)	10 (2%)	7	18
5	C	389/429 (91%)	356 (92%)	25 (6%)	8 (2%)	9	23
5	D	400/429 (93%)	361 (90%)	28 (7%)	11 (3%)	6	15
All	All	1586/1716 (92%)	1425 (90%)	121 (8%)	40 (2%)	7	18

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	152	GLU
4	A	267	SER
4	A	375	LYS
4	B	152	GLU
4	B	375	LYS

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	
4	A	364/388 (94%)	357 (98%)	7 (2%)	65	88
4	B	376/388 (97%)	367 (98%)	9 (2%)	57	85
5	C	364/387 (94%)	359 (99%)	5 (1%)	74	92
5	D	370/387 (96%)	366 (99%)	4 (1%)	80	94
All	All	1474/1550 (95%)	1449 (98%)	25 (2%)	68	90

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	282	SER
4	B	317	MET
5	D	317	MET
4	B	305	HIS
4	B	332	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	345	HIS
5	C	61	ASN
5	D	309	HIS
4	B	409	GLN
4	B	428	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PTR	C	343	1,5	11,15,17	1.95	3 (27%)	13,19,24	1.04	1 (7%)
5	PTR	D	343	1,5	11,15,17	1.85	3 (27%)	13,19,24	1.07	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PTR	C	343	1,5	-	0/6/10/13	0/1/1/1
5	PTR	D	343	1,5	-	0/6/10/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	343	PTR	CE1-CZ	2.08	1.42	1.38
5	D	343	PTR	CE2-CD2	2.22	1.42	1.38
5	C	343	PTR	CE2-CD2	2.26	1.42	1.38
5	C	343	PTR	CE1-CD1	2.79	1.43	1.38
5	C	343	PTR	OH-CZ	4.01	1.46	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	343	PTR	O-C-CA	-2.22	119.70	125.49
5	D	343	PTR	CD2-CE2-CZ	-2.06	117.14	119.74
5	D	343	PTR	O-C-CA	-2.00	120.27	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	343	PTR	1	0
5	D	343	PTR	6	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	2PO	H	513	3	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	2PO	H	513	3	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	513	2PO	2	0

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	E	13/13 (100%)	0.72	0 100 100	71, 106, 117, 124	0
1	F	13/13 (100%)	-0.98	0 100 100	34, 36, 46, 57	0
2	I	20/20 (100%)	0.70	2 (10%) 9 7	65, 109, 135, 137	0
2	J	20/20 (100%)	-0.39	0 100 100	27, 56, 86, 99	0
3	G	33/33 (100%)	-0.23	0 100 100	25, 79, 101, 102	0
3	H	33/33 (100%)	-0.15	0 100 100	33, 75, 127, 136	0
4	A	400/429 (93%)	1.56	109 (27%) 1 1	66, 125, 165, 177	0
4	B	413/429 (96%)	-0.00	22 (5%) 30 28	21, 48, 107, 133	0
5	C	399/429 (93%)	0.56	43 (10%) 8 6	46, 85, 141, 157	0
5	D	408/429 (95%)	0.01	18 (4%) 38 37	25, 55, 94, 122	0
All	All	1752/1848 (94%)	0.48	194 (11%) 7 5	21, 74, 149, 177	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	32	ALA	7.9
4	A	25	ARG	7.3
4	A	268	ASN	7.2
4	A	42	CYS	6.8
4	A	405	GLY	6.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
5	PTR	D	343	15/17	0.89	0.20	-	71,78,80,80	0
5	PTR	C	343	15/17	0.98	0.13	-	38,41,45,48	0

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
6	2PO	H	513	4/4	0.93	0.20	0.92	85,85,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.