



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 10:01 am BST

PDB ID : 1FLO
Title : FLP Recombinase-Holliday Junction Complex I
Authors : Chen, Y.; Narendra, U.; Iype, L.E.; Cox, M.M.; Rice, P.A.
Deposited on : 2000-08-14
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

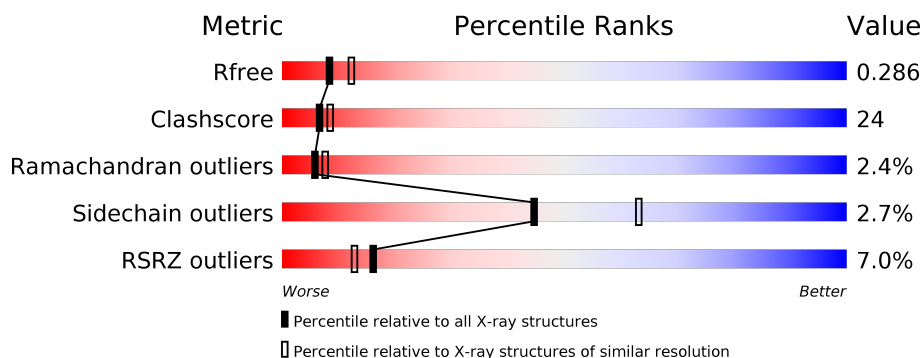
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	13	<div> <div></div> <div>46%</div> <div>54%</div> </div>
1	G	13	<div> <div></div> <div>38%</div> <div>62%</div> </div>
1	I	13	<div> <div></div> <div>23%</div> <div>77%</div> </div>
1	K	13	<div> <div></div> <div>23%</div> <div>77%</div> </div>
2	F	20	<div> <div></div> <div>45%</div> <div>50%</div> <div>5%</div> </div>
2	H	20	<div> <div></div> <div>55%</div> <div>40%</div> <div>5%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	20	<div><div></div><div>20%75%5%</div></div>
2	L	20	<div><div></div><div>25%70%5%</div></div>
3	A	422	<div><div></div><div>3%65%27%. .</div></div>
3	B	422	<div><div></div><div>7%66%28%. .</div></div>
3	C	422	<div><div></div><div>7%50%43%. .</div></div>
3	D	422	<div><div></div><div>12%48%44%. .</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16064 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 SYMMETRIZED FRT DNA SITES.

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

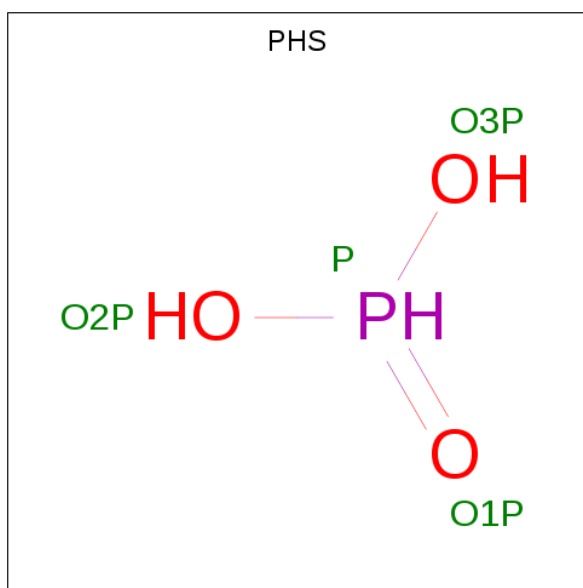
- Molecule 2 is a DNA chain called SYMMETRIZED FRT DNA SITES.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	20	Total	C	N	O	P	0	0	0
			410	198	78	115	19			
2	H	20	Total	C	N	O	P	0	0	0
			395	189	75	112	19			
2	J	19	Total	C	N	O	P	0	0	0
			391	189	75	109	18			
2	L	19	Total	C	N	O	P	0	0	0
			391	189	75	109	18			

- Molecule 3 is a protein called FLP RECOMBINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	405	Total	C	N	O	S	0	0	0
			3297	2128	553	605	11			
3	B	408	Total	C	N	O	S	0	0	0
			3323	2141	564	607	11			
3	C	404	Total	C	N	O	S	0	0	0
			3304	2133	560	600	11			
3	D	405	Total	C	N	O	S	0	0	0
			3308	2135	560	602	11			

- Molecule 4 is PHOSPHONIC ACID (three-letter code: PHS) (formula: $\text{H}_3\text{O}_3\text{P}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total O P 4 3 1	0	0
4	G	1	Total O P 4 3 1	0	0
4	I	1	Total O P 4 3 1	0	0
4	K	1	Total O P 4 3 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	10	Total O 10 10	0	0
5	F	10	Total O 10 10	0	0
5	G	3	Total O 3 3	0	0
5	H	6	Total O 6 6	0	0
5	L	1	Total O 1 1	0	0
5	A	103	Total O 103 103	0	0
5	B	38	Total O 38 38	0	0

Continued on next page...

Continued from previous page...

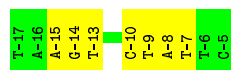
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	16	Total 16	O 16	0	0
5	D	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

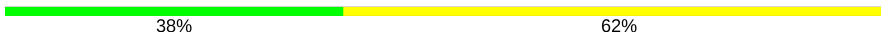
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

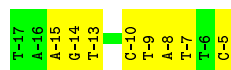
- Molecule 1: SYMMETRIZED FRT DNA SITES

Chain E: 



- Molecule 1: SYMMETRIZED FRT DNA SITES

Chain G: 



- Molecule 1: SYMMETRIZED FRT DNA SITES

Chain I: 



- Molecule 1: SYMMETRIZED FRT DNA SITES

Chain K: 



- Molecule 2: SYMMETRIZED FRT DNA SITES

Chain F: 

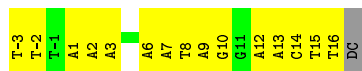


- Molecule 2: SYMMETRIZED FRT DNA SITES

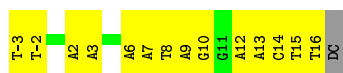
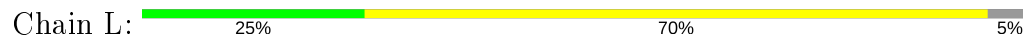
Chain H: 



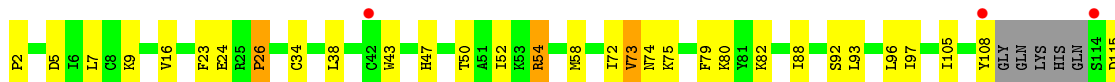
• Molecule 2: SYMMETRIZED FRT DNA SITES



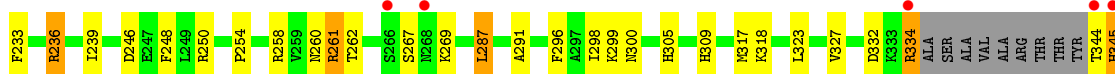
• Molecule 2: SYMMETRIZED FRT DNA SITES



• Molecule 3: FLP RECOMBINASE

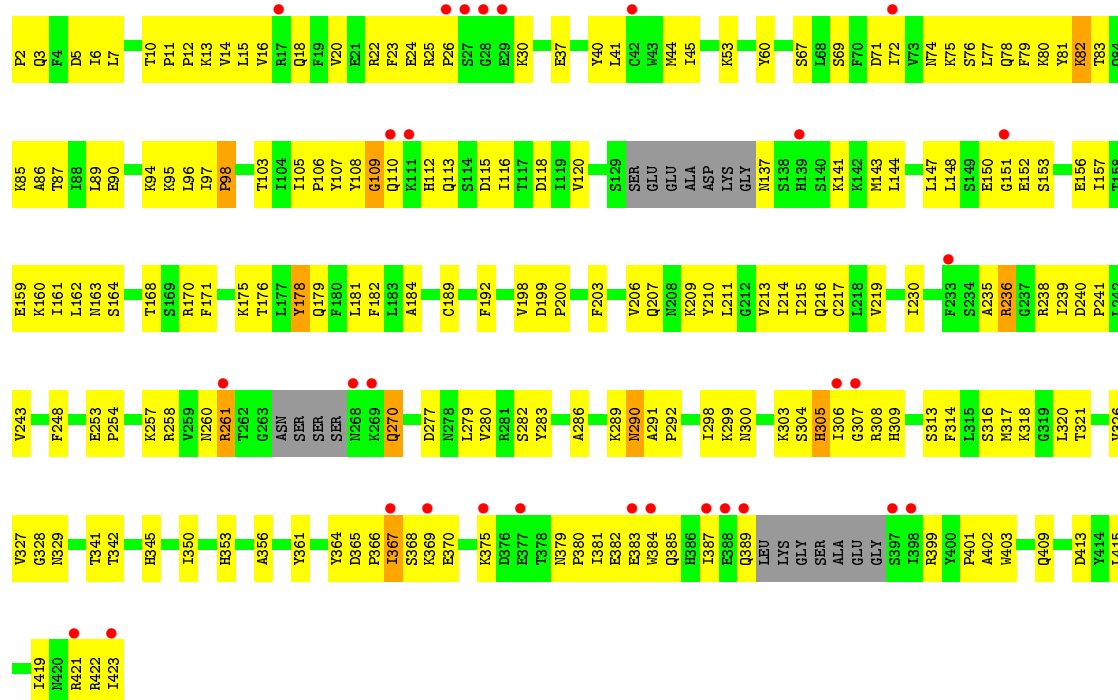


• Molecule 3: FLP RECOMBINASE

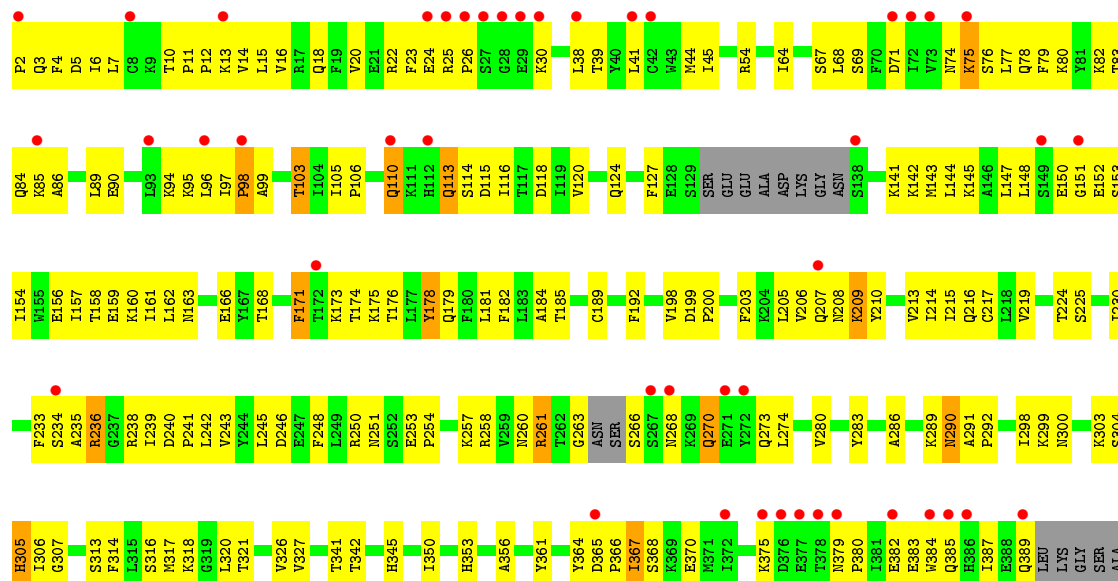




• Molecule 3: FLP RECOMBINASE



• Molecule 3: FLP RECOMBINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.48 Å 180.18 Å 98.60 Å 90.00° 97.02° 90.00°	Depositor
Resolution (Å)	15.00 – 2.65 22.52 – 2.60	Depositor EDS
% Data completeness (in resolution range)	88.5 (15.00-2.65) 87.0 (22.52-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.60 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.249 , 0.297 0.239 , 0.286	Depositor DCC
R_{free} test set	7133 reflections (9.15%)	wwPDB-VP
Wilson B-factor (Å ²)	56.4	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16064	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

5.1 Standard geometry

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

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	0.67	0/288	0.95	0/442
1	G	0.53	0/288	0.93	0/442
1	I	0.44	0/288	0.88	0/442
1	K	0.41	0/288	0.82	0/442
2	F	0.68	0/461	0.89	1/710 (0.1%)
2	H	0.55	0/444	0.86	0/685
2	J	0.45	0/440	0.82	0/678
2	L	0.40	0/440	0.78	0/678
3	A	0.48	0/3370	0.65	0/4551
3	B	0.39	0/3397	0.63	1/4585 (0.0%)
3	C	0.36	0/3378	0.58	0/4563
3	D	0.36	0/3382	0.57	0/4568
All	All	0.43	0/16464	0.67	2/22786 (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
2	H	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	110	GLN	N-CA-C	-5.71	95.58	111.00
2	F	7	DA	N9-C1'-C2'	-5.32	102.50	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	7	DA	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	12	0
1	G	259	0	150	13	0
1	I	259	0	150	10	0
1	K	259	0	150	13	0
2	F	410	0	228	14	0
2	H	395	0	216	13	0
2	J	391	0	217	25	0
2	L	391	0	217	25	0
3	A	3297	0	3339	121	0
3	B	3323	0	3369	129	0
3	C	3304	0	3350	199	0
3	D	3308	0	3354	202	0
4	E	4	0	0	1	0
4	G	4	0	0	0	0
4	I	4	0	0	0	0
4	K	4	0	0	0	0
5	A	103	0	0	7	0
5	B	38	0	0	1	0
5	C	16	0	0	7	0
5	D	6	0	0	0	0
5	E	10	0	0	1	0
5	F	10	0	0	1	0
5	G	3	0	0	0	0
5	H	6	0	0	0	0
5	L	1	0	0	1	0
All	All	16064	0	14890	724	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 24.

The worst 5 of 724 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:D:399:ARG:HH22	3:D:419:ILE:HG21	1.15	1.09
2:J:15:DT:H2"	2:J:16:DT:H5"	1.36	1.07
3:C:83:THR:HG22	3:C:85:LYS:H	1.20	1.07
3:A:148:LEU:HD12	3:D:345:HIS:HB2	1.41	1.03
3:D:83:THR:HG22	3:D:85:LYS:H	1.23	1.02

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	397/422 (94%)	361 (91%)	30 (8%)	6 (2%)	10	15
3	B	402/422 (95%)	362 (90%)	34 (8%)	6 (2%)	10	15
3	C	396/422 (94%)	344 (87%)	41 (10%)	11 (3%)	5	6
3	D	397/422 (94%)	327 (82%)	55 (14%)	15 (4%)	3	3
All	All	1592/1688 (94%)	1394 (88%)	160 (10%)	38 (2%)	6	7

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	150	GLU
3	A	377	GLU
3	A	389	GLN
3	B	114	SER
3	B	150	GLU

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	370/382 (97%)	355 (96%)	15 (4%)	30	46
3	B	372/382 (97%)	362 (97%)	10 (3%)	44	63
3	C	369/382 (97%)	363 (98%)	6 (2%)	62	78
3	D	370/382 (97%)	361 (98%)	9 (2%)	49	67
All	All	1481/1528 (97%)	1441 (97%)	40 (3%)	44	63

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	261	ARG
3	B	345	HIS
3	D	268	ASN
3	B	305	HIS
3	B	346	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	197	ASN
3	B	309	HIS
3	D	325	ASN
3	B	216	GLN
3	B	264	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands 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	$\# Z > 2$
4	PHS	I	-4	1	0,3,3	0.00	-	0,3,3	0.00	-
4	PHS	G	-4	1	0,3,3	0.00	-	0,3,3	0.00	-
4	PHS	E	-4	1	0,3,3	0.00	-	0,3,3	0.00	-
4	PHS	K	-4	1	0,3,3	0.00	-	0,3,3	0.00	-

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	-4	PHS	1	0

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	13/13 (100%)	-0.76	0	100	100	33, 38, 50, 51	0
1	G	13/13 (100%)	-0.81	0	100	100	50, 57, 69, 83	0
1	I	13/13 (100%)	-0.66	0	100	100	58, 75, 85, 99	0
1	K	13/13 (100%)	-0.28	0	100	100	65, 88, 98, 100	0
2	F	20/20 (100%)	-0.64	0	100	100	25, 48, 79, 89	0
2	H	20/20 (100%)	-0.53	0	100	100	46, 58, 84, 100	0
2	J	19/20 (95%)	-0.09	0	100	100	39, 72, 98, 99	0
2	L	19/20 (95%)	0.09	0	100	100	57, 80, 101, 101	0
3	A	405/422 (95%)	-0.14	14 (3%)	44	40	13, 47, 100, 103	0
3	B	408/422 (96%)	0.21	28 (6%)	16	13	32, 66, 102, 103	0
3	C	404/422 (95%)	0.25	30 (7%)	14	12	40, 77, 102, 103	0
3	D	405/422 (95%)	0.61	50 (12%)	4	2	35, 94, 103, 103	0
All	All	1752/1820 (96%)	0.19	122 (6%)	16	13	13, 73, 102, 103	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	109	GLY	11.8
3	B	423	ILE	10.7
3	D	28	GLY	7.7
3	B	392	GLY	6.8
3	B	112	HIS	5.9

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](#)

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(\AA^2)	Q<0.9
4	PHS	G	-4	4/4	0.98	0.12	42,43,60,61	0
4	PHS	E	-4	4/4	0.98	0.18	26,34,48,50	0
4	PHS	K	-4	4/4	0.98	0.10	51,57,60,64	0
4	PHS	I	-4	4/4	0.99	0.10	53,55,56,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.