Full wwPDB X-ray Structure Validation Report (i)

Jan 23, 2017 – 10:42 PM EST

PDB ID	:	5HXY
Title	:	Crystal structure of XerA recombinase
Authors	:	Hwang, K.Y.; Nam, K.H.
Deposited on	:	2016-01-31
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

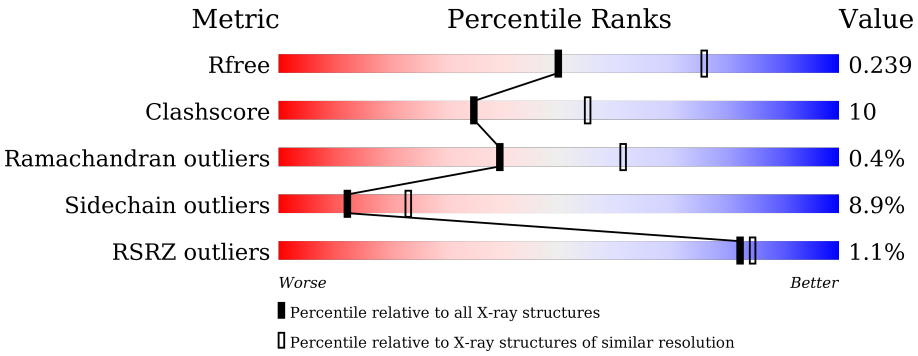
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 <=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	317	66% 19% 12%
1	B	317	65% 19% 13%
1	C	317	71% 13% 13%
1	D	317	63% 19% 14%
1	E	317	67% 20% 12%
1	F	317	58% 23% 15%

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
2	PO4	A	301	-	-	X	-
2	PO4	A	302	-	-	-	X
2	PO4	A	304	-	-	X	-
2	PO4	B	301	-	-	X	X
2	PO4	C	302	-	-	-	X
2	PO4	C	303	-	-	X	-
2	PO4	D	301	-	-	X	X
2	PO4	F	302	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14067 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 protein called Tyrosine recombinase XerA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	Se	0	0	0
			2283	1446	406	420	2	9			
1	B	275	Total	C	N	O	S	Se	0	0	0
			2246	1424	396	415	2	9			
1	C	277	Total	C	N	O	S	Se	0	0	0
			2266	1436	402	417	2	9			
1	D	274	Total	C	N	O	S	Se	0	0	0
			2234	1417	396	410	2	9			
1	E	280	Total	C	N	O	S	Se	0	0	0
			2283	1446	406	420	2	9			
1	F	268	Total	C	N	O	S	Se	0	0	0
			2189	1389	387	402	2	9			

There are 204 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MSE	-	expression tag	UNP Q9HIM5
A	-32	GLY	-	expression tag	UNP Q9HIM5
A	-31	SER	-	expression tag	UNP Q9HIM5
A	-30	SER	-	expression tag	UNP Q9HIM5
A	-29	HIS	-	expression tag	UNP Q9HIM5
A	-28	HIS	-	expression tag	UNP Q9HIM5
A	-27	HIS	-	expression tag	UNP Q9HIM5
A	-26	HIS	-	expression tag	UNP Q9HIM5
A	-25	HIS	-	expression tag	UNP Q9HIM5
A	-24	HIS	-	expression tag	UNP Q9HIM5
A	-23	SER	-	expression tag	UNP Q9HIM5
A	-22	SER	-	expression tag	UNP Q9HIM5
A	-21	GLY	-	expression tag	UNP Q9HIM5
A	-20	LEU	-	expression tag	UNP Q9HIM5
A	-19	VAL	-	expression tag	UNP Q9HIM5
A	-18	PRO	-	expression tag	UNP Q9HIM5
A	-17	ARG	-	expression tag	UNP Q9HIM5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLY	-	expression tag	UNP Q9HIM5
A	-15	SER	-	expression tag	UNP Q9HIM5
A	-14	HIS	-	expression tag	UNP Q9HIM5
A	-13	MSE	-	expression tag	UNP Q9HIM5
A	-12	ALA	-	expression tag	UNP Q9HIM5
A	-11	SER	-	expression tag	UNP Q9HIM5
A	-10	MSE	-	expression tag	UNP Q9HIM5
A	-9	THR	-	expression tag	UNP Q9HIM5
A	-8	GLY	-	expression tag	UNP Q9HIM5
A	-7	GLY	-	expression tag	UNP Q9HIM5
A	-6	GLN	-	expression tag	UNP Q9HIM5
A	-5	GLN	-	expression tag	UNP Q9HIM5
A	-4	MSE	-	expression tag	UNP Q9HIM5
A	-3	GLY	-	expression tag	UNP Q9HIM5
A	-2	ARG	-	expression tag	UNP Q9HIM5
A	-1	GLY	-	expression tag	UNP Q9HIM5
A	0	SER	-	expression tag	UNP Q9HIM5
B	-33	MSE	-	expression tag	UNP Q9HIM5
B	-32	GLY	-	expression tag	UNP Q9HIM5
B	-31	SER	-	expression tag	UNP Q9HIM5
B	-30	SER	-	expression tag	UNP Q9HIM5
B	-29	HIS	-	expression tag	UNP Q9HIM5
B	-28	HIS	-	expression tag	UNP Q9HIM5
B	-27	HIS	-	expression tag	UNP Q9HIM5
B	-26	HIS	-	expression tag	UNP Q9HIM5
B	-25	HIS	-	expression tag	UNP Q9HIM5
B	-24	HIS	-	expression tag	UNP Q9HIM5
B	-23	SER	-	expression tag	UNP Q9HIM5
B	-22	SER	-	expression tag	UNP Q9HIM5
B	-21	GLY	-	expression tag	UNP Q9HIM5
B	-20	LEU	-	expression tag	UNP Q9HIM5
B	-19	VAL	-	expression tag	UNP Q9HIM5
B	-18	PRO	-	expression tag	UNP Q9HIM5
B	-17	ARG	-	expression tag	UNP Q9HIM5
B	-16	GLY	-	expression tag	UNP Q9HIM5
B	-15	SER	-	expression tag	UNP Q9HIM5
B	-14	HIS	-	expression tag	UNP Q9HIM5
B	-13	MSE	-	expression tag	UNP Q9HIM5
B	-12	ALA	-	expression tag	UNP Q9HIM5
B	-11	SER	-	expression tag	UNP Q9HIM5
B	-10	MSE	-	expression tag	UNP Q9HIM5
B	-9	THR	-	expression tag	UNP Q9HIM5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP Q9HIM5
B	-7	GLY	-	expression tag	UNP Q9HIM5
B	-6	GLN	-	expression tag	UNP Q9HIM5
B	-5	GLN	-	expression tag	UNP Q9HIM5
B	-4	MSE	-	expression tag	UNP Q9HIM5
B	-3	GLY	-	expression tag	UNP Q9HIM5
B	-2	ARG	-	expression tag	UNP Q9HIM5
B	-1	GLY	-	expression tag	UNP Q9HIM5
B	0	SER	-	expression tag	UNP Q9HIM5
C	-33	MSE	-	expression tag	UNP Q9HIM5
C	-32	GLY	-	expression tag	UNP Q9HIM5
C	-31	SER	-	expression tag	UNP Q9HIM5
C	-30	SER	-	expression tag	UNP Q9HIM5
C	-29	HIS	-	expression tag	UNP Q9HIM5
C	-28	HIS	-	expression tag	UNP Q9HIM5
C	-27	HIS	-	expression tag	UNP Q9HIM5
C	-26	HIS	-	expression tag	UNP Q9HIM5
C	-25	HIS	-	expression tag	UNP Q9HIM5
C	-24	HIS	-	expression tag	UNP Q9HIM5
C	-23	SER	-	expression tag	UNP Q9HIM5
C	-22	SER	-	expression tag	UNP Q9HIM5
C	-21	GLY	-	expression tag	UNP Q9HIM5
C	-20	LEU	-	expression tag	UNP Q9HIM5
C	-19	VAL	-	expression tag	UNP Q9HIM5
C	-18	PRO	-	expression tag	UNP Q9HIM5
C	-17	ARG	-	expression tag	UNP Q9HIM5
C	-16	GLY	-	expression tag	UNP Q9HIM5
C	-15	SER	-	expression tag	UNP Q9HIM5
C	-14	HIS	-	expression tag	UNP Q9HIM5
C	-13	MSE	-	expression tag	UNP Q9HIM5
C	-12	ALA	-	expression tag	UNP Q9HIM5
C	-11	SER	-	expression tag	UNP Q9HIM5
C	-10	MSE	-	expression tag	UNP Q9HIM5
C	-9	THR	-	expression tag	UNP Q9HIM5
C	-8	GLY	-	expression tag	UNP Q9HIM5
C	-7	GLY	-	expression tag	UNP Q9HIM5
C	-6	GLN	-	expression tag	UNP Q9HIM5
C	-5	GLN	-	expression tag	UNP Q9HIM5
C	-4	MSE	-	expression tag	UNP Q9HIM5
C	-3	GLY	-	expression tag	UNP Q9HIM5
C	-2	ARG	-	expression tag	UNP Q9HIM5
C	-1	GLY	-	expression tag	UNP Q9HIM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	expression tag	UNP Q9HIM5
D	-33	MSE	-	expression tag	UNP Q9HIM5
D	-32	GLY	-	expression tag	UNP Q9HIM5
D	-31	SER	-	expression tag	UNP Q9HIM5
D	-30	SER	-	expression tag	UNP Q9HIM5
D	-29	HIS	-	expression tag	UNP Q9HIM5
D	-28	HIS	-	expression tag	UNP Q9HIM5
D	-27	HIS	-	expression tag	UNP Q9HIM5
D	-26	HIS	-	expression tag	UNP Q9HIM5
D	-25	HIS	-	expression tag	UNP Q9HIM5
D	-24	HIS	-	expression tag	UNP Q9HIM5
D	-23	SER	-	expression tag	UNP Q9HIM5
D	-22	SER	-	expression tag	UNP Q9HIM5
D	-21	GLY	-	expression tag	UNP Q9HIM5
D	-20	LEU	-	expression tag	UNP Q9HIM5
D	-19	VAL	-	expression tag	UNP Q9HIM5
D	-18	PRO	-	expression tag	UNP Q9HIM5
D	-17	ARG	-	expression tag	UNP Q9HIM5
D	-16	GLY	-	expression tag	UNP Q9HIM5
D	-15	SER	-	expression tag	UNP Q9HIM5
D	-14	HIS	-	expression tag	UNP Q9HIM5
D	-13	MSE	-	expression tag	UNP Q9HIM5
D	-12	ALA	-	expression tag	UNP Q9HIM5
D	-11	SER	-	expression tag	UNP Q9HIM5
D	-10	MSE	-	expression tag	UNP Q9HIM5
D	-9	THR	-	expression tag	UNP Q9HIM5
D	-8	GLY	-	expression tag	UNP Q9HIM5
D	-7	GLY	-	expression tag	UNP Q9HIM5
D	-6	GLN	-	expression tag	UNP Q9HIM5
D	-5	GLN	-	expression tag	UNP Q9HIM5
D	-4	MSE	-	expression tag	UNP Q9HIM5
D	-3	GLY	-	expression tag	UNP Q9HIM5
D	-2	ARG	-	expression tag	UNP Q9HIM5
D	-1	GLY	-	expression tag	UNP Q9HIM5
D	0	SER	-	expression tag	UNP Q9HIM5
E	-33	MSE	-	expression tag	UNP Q9HIM5
E	-32	GLY	-	expression tag	UNP Q9HIM5
E	-31	SER	-	expression tag	UNP Q9HIM5
E	-30	SER	-	expression tag	UNP Q9HIM5
E	-29	HIS	-	expression tag	UNP Q9HIM5
E	-28	HIS	-	expression tag	UNP Q9HIM5
E	-27	HIS	-	expression tag	UNP Q9HIM5

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-26	HIS	-	expression tag	UNP Q9HIM5
E	-25	HIS	-	expression tag	UNP Q9HIM5
E	-24	HIS	-	expression tag	UNP Q9HIM5
E	-23	SER	-	expression tag	UNP Q9HIM5
E	-22	SER	-	expression tag	UNP Q9HIM5
E	-21	GLY	-	expression tag	UNP Q9HIM5
E	-20	LEU	-	expression tag	UNP Q9HIM5
E	-19	VAL	-	expression tag	UNP Q9HIM5
E	-18	PRO	-	expression tag	UNP Q9HIM5
E	-17	ARG	-	expression tag	UNP Q9HIM5
E	-16	GLY	-	expression tag	UNP Q9HIM5
E	-15	SER	-	expression tag	UNP Q9HIM5
E	-14	HIS	-	expression tag	UNP Q9HIM5
E	-13	MSE	-	expression tag	UNP Q9HIM5
E	-12	ALA	-	expression tag	UNP Q9HIM5
E	-11	SER	-	expression tag	UNP Q9HIM5
E	-10	MSE	-	expression tag	UNP Q9HIM5
E	-9	THR	-	expression tag	UNP Q9HIM5
E	-8	GLY	-	expression tag	UNP Q9HIM5
E	-7	GLY	-	expression tag	UNP Q9HIM5
E	-6	GLN	-	expression tag	UNP Q9HIM5
E	-5	GLN	-	expression tag	UNP Q9HIM5
E	-4	MSE	-	expression tag	UNP Q9HIM5
E	-3	GLY	-	expression tag	UNP Q9HIM5
E	-2	ARG	-	expression tag	UNP Q9HIM5
E	-1	GLY	-	expression tag	UNP Q9HIM5
E	0	SER	-	expression tag	UNP Q9HIM5
F	-33	MSE	-	expression tag	UNP Q9HIM5
F	-32	GLY	-	expression tag	UNP Q9HIM5
F	-31	SER	-	expression tag	UNP Q9HIM5
F	-30	SER	-	expression tag	UNP Q9HIM5
F	-29	HIS	-	expression tag	UNP Q9HIM5
F	-28	HIS	-	expression tag	UNP Q9HIM5
F	-27	HIS	-	expression tag	UNP Q9HIM5
F	-26	HIS	-	expression tag	UNP Q9HIM5
F	-25	HIS	-	expression tag	UNP Q9HIM5
F	-24	HIS	-	expression tag	UNP Q9HIM5
F	-23	SER	-	expression tag	UNP Q9HIM5
F	-22	SER	-	expression tag	UNP Q9HIM5
F	-21	GLY	-	expression tag	UNP Q9HIM5
F	-20	LEU	-	expression tag	UNP Q9HIM5
F	-19	VAL	-	expression tag	UNP Q9HIM5

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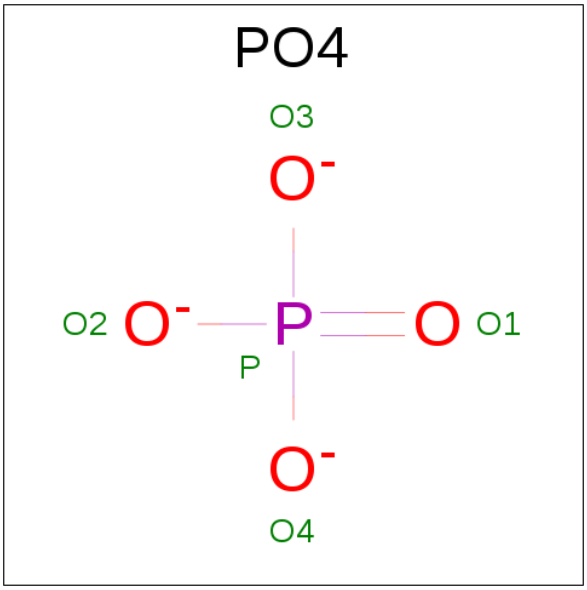
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	PRO	-	expression tag	UNP Q9HIM5
F	-17	ARG	-	expression tag	UNP Q9HIM5
F	-16	GLY	-	expression tag	UNP Q9HIM5
F	-15	SER	-	expression tag	UNP Q9HIM5
F	-14	HIS	-	expression tag	UNP Q9HIM5
F	-13	MSE	-	expression tag	UNP Q9HIM5
F	-12	ALA	-	expression tag	UNP Q9HIM5
F	-11	SER	-	expression tag	UNP Q9HIM5
F	-10	MSE	-	expression tag	UNP Q9HIM5
F	-9	THR	-	expression tag	UNP Q9HIM5
F	-8	GLY	-	expression tag	UNP Q9HIM5
F	-7	GLY	-	expression tag	UNP Q9HIM5
F	-6	GLN	-	expression tag	UNP Q9HIM5
F	-5	GLN	-	expression tag	UNP Q9HIM5
F	-4	MSE	-	expression tag	UNP Q9HIM5
F	-3	GLY	-	expression tag	UNP Q9HIM5
F	-2	ARG	-	expression tag	UNP Q9HIM5
F	-1	GLY	-	expression tag	UNP Q9HIM5
F	0	SER	-	expression tag	UNP Q9HIM5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

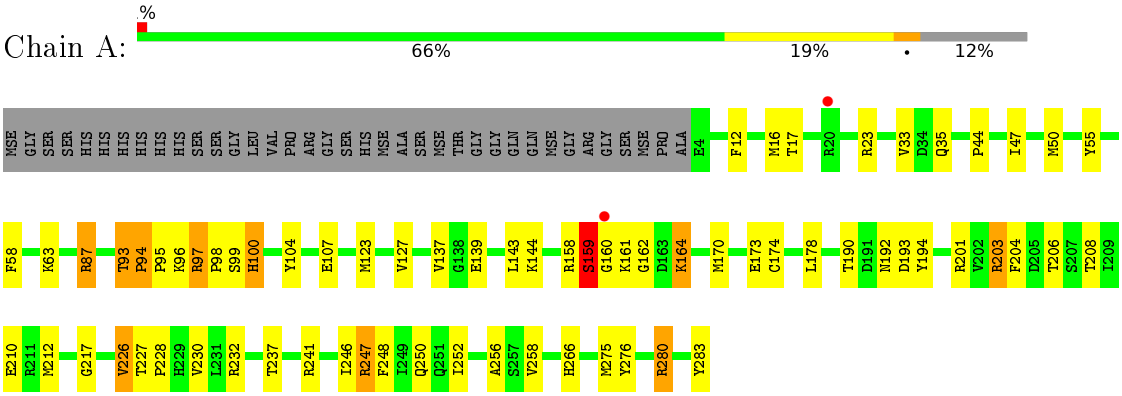
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total O 62 62	0	0
3	B	98	Total O 98 98	0	0
3	C	113	Total O 113 113	0	0
3	D	56	Total O 56 56	0	0
3	E	115	Total O 115 115	0	0
3	F	47	Total O 47 47	0	0

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.

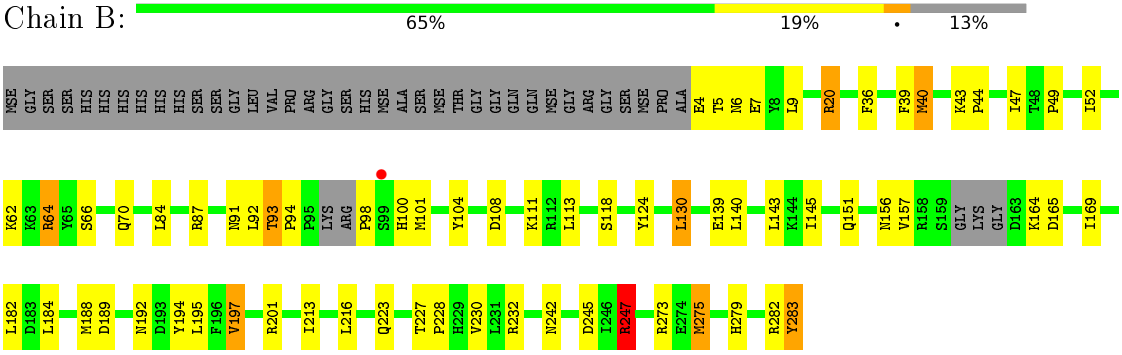
- Molecule 1: Tyrosine recombinase XerA

Chain A:



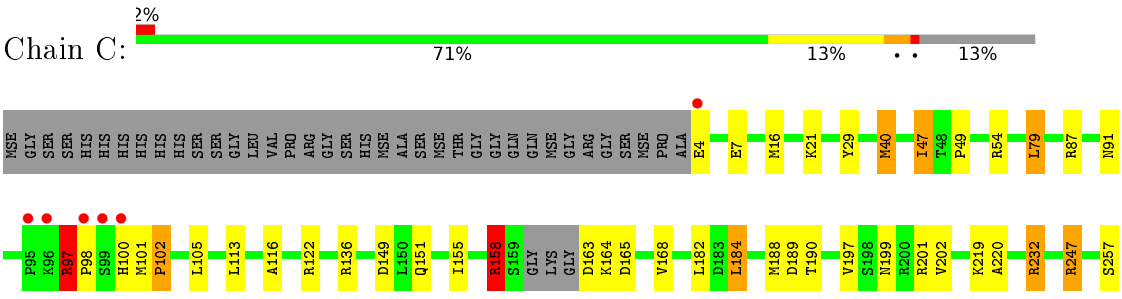
- Molecule 1: Tyrosine recombinase XerA

Chain B:



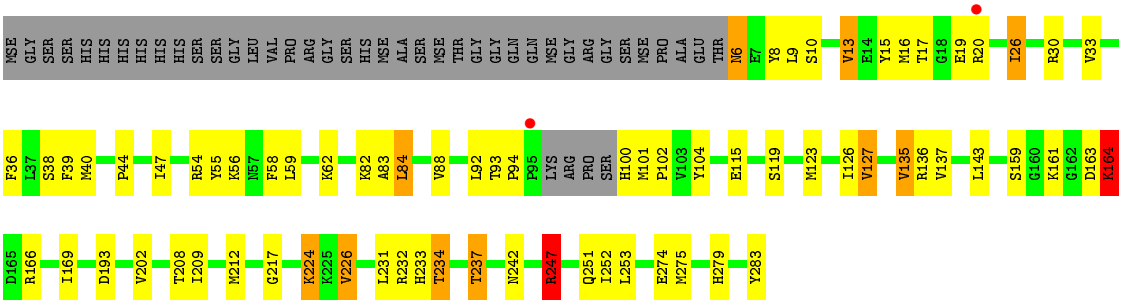
- Molecule 1: Tyrosine recombinase XerA

Chain C:



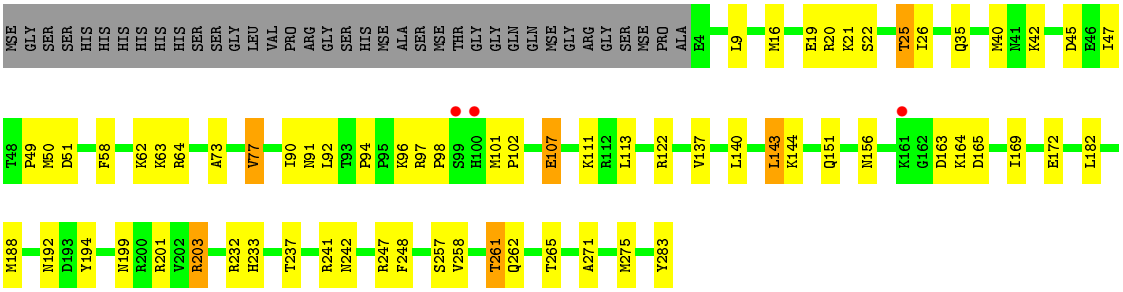
• Molecule 1: Tyrosine recombinase XerA

Chain D:



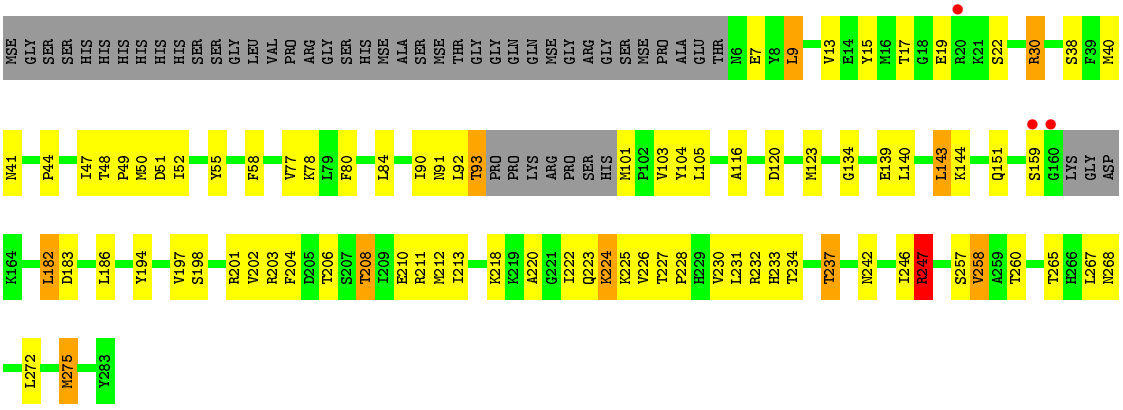
• Molecule 1: Tyrosine recombinase XerA

Chain E:



• Molecule 1: Tyrosine recombinase XerA

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.86Å 105.97Å 115.59Å 90.00° 110.01° 90.00°	Depositor
Resolution (Å)	47.66 – 2.50 47.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.66-2.50) 95.3 (47.62-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.188 , 0.243 0.191 , 0.239	Depositor DCC
R_{free} test set	3474 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14067	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4

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	0.66	0/2314	0.87	4/3101 (0.1%)
1	B	0.73	0/2275	0.89	2/3048 (0.1%)
1	C	0.75	0/2296	0.94	8/3077 (0.3%)
1	D	0.65	0/2263	0.87	2/3031 (0.1%)
1	E	0.75	0/2314	0.92	3/3101 (0.1%)
1	F	0.63	0/2215	0.85	2/2965 (0.1%)
All	All	0.70	0/13677	0.89	21/18323 (0.1%)

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	1	2
1	D	1	1
1	E	0	1
All	All	2	4

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	232	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	A	159	SER	N-CA-C	6.82	129.42	111.00
1	D	247	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	B	247	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	B	245	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	280	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	203	ARG	NE-CZ-NH1	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	282	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	E	232	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	97	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	164	LYS	N-CA-C	5.55	125.98	111.00
1	A	280	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	158	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	F	247	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	93	THR	C-N-CD	-5.31	108.92	120.60
1	C	232	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	149	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	282	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	F	258	VAL	CB-CA-C	-5.14	101.63	111.40
1	C	54	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	E	45	ASP	CB-CG-OD1	5.04	122.84	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	159	SER	CA
1	D	164	LYS	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	HIS	Peptide
1	A	93	THR	Peptide
1	D	163	ASP	Peptide
1	E	163	ASP	Peptide

5.2 Too-close contacts (i)

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	2283	0	2333	54	0
1	B	2246	0	2287	52	0
1	C	2266	0	2313	44	0
1	D	2234	0	2281	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2283	0	2333	47	0
1	F	2189	0	2239	65	0
2	A	20	0	0	6	0
2	B	10	0	0	4	0
2	C	15	0	0	3	0
2	D	10	0	0	3	0
2	E	10	0	0	1	0
2	F	10	0	0	0	0
3	A	62	0	0	4	0
3	B	98	0	0	2	1
3	C	113	0	0	2	0
3	D	56	0	0	3	0
3	E	115	0	0	6	0
3	F	47	0	0	1	0
All	All	14067	0	13786	270	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 10.

All (270) 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)
1:A:170:MSE:HE2	1:A:174:CYS:SG	1.99	1.02
2:D:302:PO4:O1	3:D:401:HOH:O	1.78	1.01
1:C:16:MSE:HE2	1:C:21:LYS:HD2	1.40	0.99
1:D:208:THR:HG22	1:D:212:MSE:HE2	1.46	0.97
1:B:232:ARG:NH2	2:B:301:PO4:O4	2.06	0.89
1:B:184:LEU:HD21	1:B:188:MSE:HE3	1.54	0.86
1:A:87:ARG:HG2	1:A:87:ARG:HH11	1.40	0.86
1:F:49:PRO:HB3	1:F:91:ASN:HD21	1.42	0.83
1:D:209:ILE:HA	1:D:212:MSE:HE3	1.58	0.83
1:F:123:MSE:HE1	1:F:212:MSE:SE	2.30	0.80
1:B:197:VAL:HG13	1:B:201:ARG:HA	1.64	0.80
1:A:160:GLY:HA2	1:A:161:LYS:HB2	1.64	0.79
2:B:302:PO4:O1	3:B:401:HOH:O	2.01	0.79
1:E:164:LYS:O	3:E:401:HOH:O	2.02	0.77
1:E:40:MSE:HE2	1:E:47:ILE:HD12	1.67	0.77
1:F:49:PRO:CB	1:F:91:ASN:HD21	1.97	0.77
1:B:184:LEU:CD2	1:B:188:MSE:HE3	2.15	0.76
1:F:104:TYR:CE2	1:F:237:THR:HG21	2.21	0.75
1:F:50:MSE:HA	1:F:50:MSE:HE2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:TYR:OH	1:A:203:ARG:NH1	2.20	0.74
1:F:15:TYR:CE2	1:F:19:GLU:OE2	2.41	0.73
1:D:44:PRO:HA	1:D:47:ILE:HD12	1.69	0.73
1:A:35:GLN:HE22	1:A:63:LYS:HE3	1.54	0.72
1:C:16:MSE:HE2	1:C:21:LYS:CD	2.18	0.72
1:C:165:ASP:HB3	1:E:98:PRO:HB3	1.71	0.71
1:E:90:ILE:HD12	1:E:90:ILE:H	1.55	0.71
1:D:55:TYR:O	1:D:58:PHE:HB3	1.90	0.71
1:C:189:ASP:HB2	3:C:474:HOH:O	1.93	0.68
1:B:242:ASN:O	1:C:279:HIS:HD2	1.77	0.67
1:B:283:TYR:HA	1:E:111:LYS:NZ	2.10	0.66
1:B:275:MSE:HG2	1:E:248:PHE:CE1	2.31	0.65
1:B:156:ASN:HD22	1:C:98:PRO:CD	2.08	0.65
1:A:192:ASN:HD22	1:A:194:TYR:H	1.44	0.65
1:C:40:MSE:HE2	2:C:303:PO4:O1	1.97	0.65
1:D:33:VAL:O	1:D:36:PHE:HB3	1.97	0.65
1:D:92:LEU:O	1:D:94:PRO:HD3	1.98	0.64
1:A:208:THR:HG22	1:A:212:MSE:HE3	1.80	0.64
1:A:206:THR:HG22	3:A:436:HOH:O	1.97	0.63
1:D:166:ARG:NH1	1:D:252:ILE:O	2.31	0.63
1:D:232:ARG:NH2	2:D:301:PO4:O1	2.32	0.63
1:C:16:MSE:HE1	1:C:29:TYR:CG	2.34	0.63
1:F:44:PRO:HA	1:F:47:ILE:HD12	1.81	0.63
1:B:156:ASN:HD22	1:C:98:PRO:HD2	1.65	0.62
1:C:16:MSE:HE1	1:C:29:TYR:CD2	2.34	0.62
1:C:247:ARG:NH1	1:E:262:GLN:O	2.33	0.62
1:E:241:ARG:HD3	1:E:271:ALA:HB1	1.81	0.62
1:A:161:LYS:CG	1:A:162:GLY:H	2.13	0.61
1:B:93:THR:HG23	1:B:93:THR:O	2.00	0.61
1:D:123:MSE:HE3	1:D:126:ILE:HB	1.82	0.61
1:F:208:THR:O	1:F:212:MSE:HE3	2.00	0.61
1:D:104:TYR:CE2	1:D:237:THR:HG21	2.36	0.60
1:A:170:MSE:CE	1:A:174:CYS:SG	2.83	0.60
1:A:94:PRO:HB2	1:A:95:PRO:HD2	1.84	0.60
1:D:123:MSE:O	1:D:127:VAL:HG23	2.02	0.60
1:E:40:MSE:HE1	1:E:51:ASP:HB3	1.84	0.59
1:F:104:TYR:HB2	1:F:234:THR:HG22	1.83	0.59
1:A:161:LYS:HG2	1:A:162:GLY:H	1.68	0.59
1:A:241:ARG:HA	1:A:275:MSE:HE1	1.85	0.59
1:B:93:THR:CG2	1:B:93:THR:O	2.50	0.59
1:F:208:THR:HG23	1:F:211:ARG:NH2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:MSE:CE	1:E:51:ASP:HB3	2.33	0.58
1:C:97:ARG:CG	1:C:97:ARG:HH11	2.16	0.58
1:B:36:PHE:CE1	1:B:40:MSE:HE2	2.39	0.58
1:F:105:LEU:H	1:F:234:THR:CG2	2.17	0.58
1:F:208:THR:C	1:F:212:MSE:HE3	2.24	0.58
1:F:134:GLY:O	1:F:232:ARG:HD3	2.02	0.58
1:F:40:MSE:HG2	1:F:47:ILE:HD11	1.85	0.58
1:E:107:GLU:OE2	1:E:241:ARG:NH2	2.37	0.58
1:F:208:THR:HG22	1:F:212:MSE:HE2	1.86	0.57
1:E:96:LYS:HG2	1:E:97:ARG:O	2.05	0.57
1:F:103:VAL:HG22	1:F:104:TYR:H	1.69	0.57
1:D:16:MSE:HE3	1:D:26:ILE:HG12	1.87	0.56
1:C:232:ARG:NH2	2:C:301:PO4:O4	2.37	0.56
1:B:169:ILE:HD11	1:C:272:LEU:HB3	1.88	0.56
1:D:56:LYS:NZ	3:D:405:HOH:O	2.39	0.56
1:F:7:GLU:HA	1:F:7:GLU:OE1	2.06	0.56
1:B:273:ARG:HA	1:E:169:ILE:HG12	1.87	0.56
1:A:266:HIS:CE1	1:D:251:GLN:NE2	2.73	0.56
1:E:22:SER:OG	1:E:25:THR:HG23	2.06	0.56
1:F:202:VAL:HG22	1:F:203:ARG:H	1.70	0.56
1:B:130:LEU:HD13	1:B:140:LEU:HD13	1.87	0.55
1:F:182:LEU:O	1:F:183:ASP:C	2.45	0.55
1:A:123:MSE:O	1:A:127:VAL:HG23	2.07	0.55
1:C:190:THR:HG22	1:C:201:ARG:HB3	1.89	0.55
1:C:40:MSE:HG2	1:C:47:ILE:HD11	1.88	0.55
1:A:94:PRO:CB	1:A:95:PRO:HD2	2.36	0.55
1:D:209:ILE:HD13	1:D:212:MSE:HE1	1.89	0.54
1:F:52:ILE:HD12	1:F:92:LEU:HD13	1.90	0.54
1:B:165:ASP:HB3	1:C:98:PRO:HG3	1.88	0.54
1:F:213:ILE:HG22	1:F:226:VAL:HG12	1.89	0.54
1:B:232:ARG:CZ	2:B:301:PO4:O4	2.56	0.53
1:D:13:VAL:HB	1:D:26:ILE:HD11	1.89	0.53
1:F:40:MSE:HG2	1:F:47:ILE:CD1	2.38	0.53
1:E:49:PRO:HB3	1:E:91:ASN:ND2	2.23	0.53
1:B:156:ASN:HD21	1:C:97:ARG:HG2	1.74	0.53
1:B:49:PRO:HB3	1:B:91:ASN:ND2	2.24	0.53
1:C:40:MSE:CE	2:C:303:PO4:O1	2.57	0.53
1:B:275:MSE:HG2	1:E:248:PHE:CD1	2.43	0.53
1:B:242:ASN:O	1:C:279:HIS:CD2	2.61	0.52
1:A:139:GLU:O	1:A:143:LEU:HD13	2.09	0.52
1:A:87:ARG:HG2	1:A:87:ARG:NH1	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:PHE:CE1	1:F:212:MSE:HE1	2.45	0.52
1:A:206:THR:O	1:A:210:GLU:HG3	2.10	0.52
1:A:97:ARG:HG3	1:A:98:PRO:HD2	1.92	0.52
1:B:279:HIS:HD2	1:E:242:ASN:O	1.93	0.52
1:D:15:TYR:O	1:D:19:GLU:HG2	2.10	0.51
1:F:48:THR:O	1:F:51:ASP:HB2	2.10	0.51
1:A:50:MSE:CE	1:D:193:ASP:HA	2.40	0.51
1:F:80:PHE:CE1	1:F:84:LEU:HD11	2.46	0.51
1:D:137:VAL:HG12	2:D:301:PO4:O3	2.10	0.51
1:F:40:MSE:HE3	1:F:40:MSE:HA	1.93	0.51
1:E:40:MSE:HE1	1:E:51:ASP:CG	2.31	0.51
1:D:209:ILE:HD13	1:D:212:MSE:CE	2.42	0.50
1:E:16:MSE:HE3	1:E:21:LYS:HD2	1.92	0.50
1:A:104:TYR:HA	1:A:230:VAL:HG13	1.92	0.50
1:B:283:TYR:HA	1:E:111:LYS:HZ3	1.76	0.50
1:F:104:TYR:HB2	1:F:234:THR:CG2	2.41	0.50
1:A:159:SER:OG	1:A:160:GLY:N	2.44	0.50
1:E:94:PRO:HD3	3:E:407:HOH:O	2.10	0.50
1:B:192:ASN:HD22	1:B:194:TYR:H	1.58	0.50
1:B:92:LEU:O	1:B:94:PRO:HD3	2.11	0.50
1:E:90:ILE:CD1	1:E:90:ILE:H	2.24	0.50
1:B:139:GLU:O	1:B:143:LEU:HG	2.12	0.50
1:B:232:ARG:NH2	2:B:301:PO4:P	2.84	0.50
1:E:40:MSE:HE1	1:E:51:ASP:CB	2.42	0.50
1:B:184:LEU:C	1:B:184:LEU:HD23	2.32	0.49
1:B:156:ASN:HD22	1:C:98:PRO:HD3	1.75	0.49
1:B:52:ILE:HD12	1:B:92:LEU:HD13	1.95	0.49
1:C:40:MSE:HA	1:C:40:MSE:HE3	1.95	0.49
1:A:12:PHE:CE2	1:A:33:VAL:HG21	2.48	0.49
1:C:116:ALA:CB	1:C:220:ALA:HB2	2.43	0.49
1:B:227:THR:HB	1:B:228:PRO:HD2	1.94	0.49
1:F:224:LYS:HE3	1:F:224:LYS:H	1.78	0.48
1:F:227:THR:HB	1:F:228:PRO:CD	2.43	0.48
1:E:241:ARG:HD2	3:E:498:HOH:O	2.13	0.48
1:E:16:MSE:CE	1:E:21:LYS:HD2	2.43	0.48
1:D:224:LYS:CE	1:D:224:LYS:HA	2.44	0.48
1:C:122:ARG:HH22	1:C:199:ASN:HD21	1.62	0.48
1:F:105:LEU:H	1:F:234:THR:HG22	1.79	0.48
1:A:161:LYS:HG2	1:A:162:GLY:N	2.29	0.48
1:C:16:MSE:HE3	1:C:79:LEU:HD12	1.95	0.48
1:F:55:TYR:O	1:F:58:PHE:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ILE:N	1:E:90:ILE:HD12	2.26	0.48
1:F:105:LEU:HB2	1:F:234:THR:HG21	1.96	0.48
1:F:120:ASP:C	1:F:120:ASP:OD1	2.52	0.48
1:A:44:PRO:HA	1:A:47:ILE:HD12	1.95	0.48
1:B:20:ARG:HA	1:B:20:ARG:NE	2.29	0.48
1:A:250:GLN:NE2	1:A:258:VAL:HG13	2.29	0.47
1:A:256:ALA:N	2:A:304:PO4:O2	2.40	0.47
1:C:189:ASP:CB	3:C:474:HOH:O	2.54	0.47
1:C:40:MSE:HG2	1:C:47:ILE:CG1	2.45	0.47
1:A:237:THR:HG22	3:A:440:HOH:O	2.15	0.47
1:C:122:ARG:HH22	1:C:199:ASN:ND2	2.12	0.47
1:D:54:ARG:NH1	1:F:186:LEU:O	2.39	0.47
1:F:144:LYS:HE2	1:F:194:TYR:CE1	2.50	0.47
1:A:164:LYS:HG2	3:A:451:HOH:O	2.14	0.47
1:B:247:ARG:HD2	1:C:265:THR:OG1	2.15	0.47
1:E:58:PHE:O	1:E:62:LYS:HB3	2.15	0.47
1:B:184:LEU:HD23	1:B:184:LEU:O	2.15	0.47
1:D:8:TYR:HD1	1:D:84:LEU:HD22	1.80	0.46
1:E:102:PRO:CD	3:E:506:HOH:O	2.63	0.46
1:E:73:ALA:O	1:E:77:VAL:HG12	2.15	0.46
1:B:113:LEU:HD12	1:B:216:LEU:HG	1.97	0.46
1:A:137:VAL:HG21	1:A:228:PRO:HG3	1.97	0.46
1:F:230:VAL:O	1:F:234:THR:HG23	2.14	0.46
1:A:190:THR:HG22	1:A:201:ARG:HB3	1.98	0.46
1:A:248:PHE:CD1	1:F:275:MSE:HG2	2.51	0.46
1:B:156:ASN:ND2	1:C:98:PRO:HD2	2.29	0.46
1:A:50:MSE:HE3	1:D:193:ASP:HA	1.97	0.46
1:A:99:SER:O	1:D:164:LYS:NZ	2.49	0.46
1:A:252:ILE:HD11	1:F:272:LEU:HD22	1.96	0.46
1:B:100:HIS:CD2	1:B:101:MSE:HE3	2.51	0.46
1:E:140:LEU:HA	1:E:143:LEU:HD22	1.98	0.46
1:F:198:SER:HA	1:F:204:PHE:CZ	2.52	0.45
1:C:155:ILE:HB	1:C:168:VAL:CG2	2.46	0.45
1:B:130:LEU:CD2	1:B:213:ILE:HD11	2.46	0.45
1:B:197:VAL:CG1	1:B:201:ARG:HA	2.41	0.45
1:B:283:TYR:HA	1:E:111:LYS:HZ2	1.77	0.45
1:E:16:MSE:HE3	1:E:21:LYS:CD	2.46	0.45
1:A:12:PHE:CD1	1:A:16:MSE:HE2	2.52	0.45
1:F:78:LYS:HE2	1:F:93:THR:HG22	1.98	0.45
1:A:232:ARG:NH1	2:A:301:PO4:O2	2.48	0.45
1:C:136:ARG:HA	1:C:232:ARG:NH2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ARG:HG3	1:C:97:ARG:HH11	1.82	0.45
1:E:19:GLU:OE2	3:E:402:HOH:O	2.21	0.44
1:C:4:GLU:O	1:C:7:GLU:HB3	2.16	0.44
1:D:247:ARG:NH2	3:D:406:HOH:O	2.43	0.44
1:E:42:LYS:NZ	1:E:51:ASP:OD2	2.43	0.44
1:A:217:GLY:HA3	1:A:226:VAL:HG13	1.99	0.44
1:A:256:ALA:H	2:A:304:PO4:P	2.39	0.44
1:C:257:SER:O	1:C:260:THR:HG23	2.17	0.44
1:A:17:THR:HG23	3:A:419:HOH:O	2.16	0.44
1:A:247:ARG:NH2	2:A:302:PO4:O3	2.50	0.44
1:F:103:VAL:HG22	1:F:104:TYR:N	2.33	0.44
1:C:16:MSE:CE	1:C:29:TYR:CD2	3.00	0.44
1:D:59:LEU:HD23	1:D:59:LEU:HA	1.85	0.44
1:E:192:ASN:HD22	1:E:194:TYR:H	1.66	0.44
1:E:233:HIS:HD2	1:E:237:THR:HG23	1.83	0.44
1:F:233:HIS:O	1:F:237:THR:HB	2.17	0.44
1:F:208:THR:HG22	1:F:212:MSE:CE	2.47	0.44
1:B:98:PRO:HB3	1:E:165:ASP:HB3	2.00	0.44
1:D:82:LYS:O	1:D:83:ALA:C	2.56	0.44
1:F:9:LEU:O	1:F:13:VAL:HG23	2.18	0.43
1:D:233:HIS:O	1:D:237:THR:HB	2.19	0.43
1:F:116:ALA:HB2	1:F:220:ALA:HB2	1.99	0.43
1:A:204:PHE:CE1	1:A:212:MSE:HE1	2.54	0.43
1:B:111:LYS:CE	1:C:283:TYR:HA	2.48	0.43
1:B:282:ARG:HD3	1:B:282:ARG:HA	1.62	0.43
1:F:234:THR:O	1:F:237:THR:HG22	2.18	0.43
1:A:232:ARG:HH22	2:A:301:PO4:P	2.41	0.43
1:B:145:ILE:HD13	1:B:195:LEU:HA	2.01	0.43
1:D:135:VAL:HG13	1:D:136:ARG:O	2.18	0.43
1:D:10:SER:HA	1:D:13:VAL:HG13	2.00	0.43
1:C:100:HIS:CD2	1:C:101:MSE:HE3	2.53	0.43
1:F:104:TYR:OH	1:F:268:ASN:ND2	2.52	0.43
1:C:40:MSE:HG2	1:C:47:ILE:HG12	2.00	0.43
1:D:39:PHE:CD1	1:D:39:PHE:C	2.91	0.43
1:E:203:ARG:HD2	3:E:406:HOH:O	2.18	0.43
1:F:246:ILE:HG23	1:F:247:ARG:N	2.34	0.43
1:C:49:PRO:HB3	1:C:91:ASN:ND2	2.33	0.43
1:F:49:PRO:HB3	1:F:91:ASN:ND2	2.22	0.43
1:B:43:LYS:O	1:B:44:PRO:C	2.57	0.43
1:C:40:MSE:HG2	1:C:47:ILE:CD1	2.47	0.42
1:D:279:HIS:HD2	1:F:242:ASN:O	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:206:THR:O	1:F:210:GLU:HG3	2.19	0.42
1:A:227:THR:HB	1:A:228:PRO:HD2	2.02	0.42
1:A:246:ILE:HG23	1:A:247:ARG:N	2.34	0.42
1:B:118:SER:HA	1:B:124:TYR:CD1	2.55	0.42
1:A:161:LYS:CG	1:A:162:GLY:N	2.77	0.42
1:A:247:ARG:HD2	1:F:265:THR:OG1	2.20	0.42
1:D:40:MSE:HE3	1:D:47:ILE:CG2	2.49	0.42
1:F:139:GLU:O	1:F:143:LEU:HD13	2.20	0.42
1:B:39:PHE:C	1:B:39:PHE:CD1	2.93	0.42
1:E:20:ARG:HA	1:E:20:ARG:NE	2.35	0.42
1:F:78:LYS:CE	1:F:93:THR:HG22	2.50	0.42
1:C:247:ARG:HD2	1:E:265:THR:OG1	2.20	0.41
1:F:228:PRO:O	1:F:231:LEU:N	2.53	0.41
1:B:104:TYR:HA	1:B:230:VAL:HG13	2.01	0.41
1:F:30:ARG:HG3	1:F:30:ARG:HH11	1.85	0.41
1:D:101:MSE:CB	1:D:102:PRO:HD2	2.50	0.41
1:D:231:LEU:HA	1:D:234:THR:HG23	2.02	0.41
1:E:137:VAL:HG12	2:E:302:PO4:O4	2.19	0.41
1:E:16:MSE:HB3	1:E:26:ILE:HG12	2.02	0.41
1:E:188:MSE:CE	1:E:201:ARG:HG2	2.50	0.41
1:F:237:THR:OG1	1:F:267:LEU:HD23	2.20	0.41
1:F:77:VAL:O	1:F:80:PHE:HB3	2.20	0.41
1:A:204:PHE:HE1	1:A:212:MSE:HE1	1.86	0.41
1:A:87:ARG:NH1	1:A:87:ARG:CG	2.83	0.41
1:D:217:GLY:HA3	1:D:226:VAL:CG1	2.50	0.41
1:F:223:GLN:N	1:F:224:LYS:HE3	2.35	0.41
1:E:35:GLN:HE22	1:E:63:LYS:HE2	1.85	0.41
1:B:66:SER:O	1:B:70:GLN:HG3	2.20	0.41
1:F:40:MSE:CE	3:F:418:HOH:O	2.69	0.41
1:A:193:ASP:HB3	1:F:50:MSE:HE3	2.02	0.41
1:B:4:GLU:O	1:B:7:GLU:HB3	2.19	0.41
1:C:184:LEU:HD13	1:C:188:MSE:HE3	2.02	0.41
1:B:130:LEU:HD13	1:B:140:LEU:CD1	2.50	0.41
1:F:140:LEU:HA	1:F:143:LEU:HD22	2.03	0.41
1:E:101:MSE:HE3	1:E:101:MSE:HB3	2.01	0.41
1:F:50:MSE:HA	1:F:50:MSE:CE	2.45	0.41
1:A:276:TYR:CD2	1:D:169:ILE:HB	2.56	0.40
1:D:6:ASN:HD22	1:D:6:ASN:HA	1.74	0.40
1:E:122:ARG:HH22	1:E:199:ASN:HD21	1.69	0.40
1:A:232:ARG:NH2	2:A:301:PO4:O1	2.42	0.40
1:A:55:TYR:O	1:A:58:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:VAL:O	1:F:17:THR:HG23	2.21	0.40
1:C:158:ARG:HG2	1:C:158:ARG:HH11	1.87	0.40
1:B:64:ARG:CD	3:B:477:HOH:O	2.69	0.40
1:E:258:VAL:HA	1:E:261:THR:HG23	2.04	0.40
1:F:41:ASN:O	1:F:41:ASN:CG	2.60	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)
3:B:457:HOH:O	3:B:457:HOH:O[2_555]	2.15	0.05

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	
1	A	278/317 (88%)	259 (93%)	17 (6%)	2 (1%)	26	46
1	B	269/317 (85%)	259 (96%)	10 (4%)	0	100	100
1	C	273/317 (86%)	262 (96%)	10 (4%)	1 (0%)	39	61
1	D	270/317 (85%)	256 (95%)	12 (4%)	2 (1%)	26	46
1	E	278/317 (88%)	266 (96%)	12 (4%)	0	100	100
1	F	262/317 (83%)	252 (96%)	9 (3%)	1 (0%)	39	61
All	All	1630/1902 (86%)	1554 (95%)	70 (4%)	6 (0%)	39	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	164	LYS
1	A	94	PRO
1	F	222	ILE

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Mol	Chain	Res	Type
1	A	100	HIS
1	C	102	PRO
1	D	93	THR

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
1	A	253/267 (95%)	237 (94%)	16 (6%)	22 40
1	B	250/267 (94%)	227 (91%)	23 (9%)	11 21
1	C	252/267 (94%)	230 (91%)	22 (9%)	13 24
1	D	247/267 (92%)	217 (88%)	30 (12%)	6 11
1	E	253/267 (95%)	234 (92%)	19 (8%)	17 31
1	F	242/267 (91%)	219 (90%)	23 (10%)	11 20
All	All	1497/1602 (93%)	1364 (91%)	133 (9%)	12 23

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	87	ARG
1	A	96	LYS
1	A	97	ARG
1	A	107	GLU
1	A	144	LYS
1	A	158	ARG
1	A	159	SER
1	A	164	LYS
1	A	173	GLU
1	A	178	LEU
1	A	203	ARG
1	A	226	VAL
1	A	247	ARG
1	A	280	ARG

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Mol	Chain	Res	Type
1	A	283	TYR
1	B	5	THR
1	B	6	ASN
1	B	9	LEU
1	B	20	ARG
1	B	40	MSE
1	B	47	ILE
1	B	62	LYS
1	B	64	ARG
1	B	84	LEU
1	B	87	ARG
1	B	93	THR
1	B	108	ASP
1	B	130	LEU
1	B	151	GLN
1	B	157	VAL
1	B	164	LYS
1	B	182	LEU
1	B	189	ASP
1	B	197	VAL
1	B	223	GLN
1	B	247	ARG
1	B	275	MSE
1	B	283	TYR
1	C	40	MSE
1	C	47	ILE
1	C	79	LEU
1	C	87	ARG
1	C	97	ARG
1	C	102	PRO
1	C	105	LEU
1	C	113	LEU
1	C	151	GLN
1	C	158	ARG
1	C	163	ASP
1	C	164	LYS
1	C	182	LEU
1	C	184	LEU
1	C	197	VAL
1	C	202	VAL
1	C	219	LYS
1	C	247	ARG

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Mol	Chain	Res	Type
1	C	260	THR
1	C	267	LEU
1	C	272	LEU
1	C	275	MSE
1	D	6	ASN
1	D	9	LEU
1	D	13	VAL
1	D	17	THR
1	D	20	ARG
1	D	26	ILE
1	D	30	ARG
1	D	38	SER
1	D	62	LYS
1	D	84	LEU
1	D	88	VAL
1	D	100	HIS
1	D	115	GLU
1	D	119	SER
1	D	127	VAL
1	D	135	VAL
1	D	143	LEU
1	D	159	SER
1	D	161	LYS
1	D	202	VAL
1	D	224	LYS
1	D	226	VAL
1	D	234	THR
1	D	237	THR
1	D	242	ASN
1	D	247	ARG
1	D	253	LEU
1	D	274	GLU
1	D	275	MSE
1	D	283	TYR
1	E	9	LEU
1	E	25	THR
1	E	50	MSE
1	E	64	ARG
1	E	77	VAL
1	E	92	LEU
1	E	107	GLU
1	E	113	LEU

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Mol	Chain	Res	Type
1	E	143	LEU
1	E	144	LYS
1	E	151	GLN
1	E	156	ASN
1	E	172	GLU
1	E	182	LEU
1	E	247	ARG
1	E	257	SER
1	E	261	THR
1	E	275	MSE
1	E	283	TYR
1	F	9	LEU
1	F	22	SER
1	F	30	ARG
1	F	38	SER
1	F	90	ILE
1	F	93	THR
1	F	101	MSE
1	F	143	LEU
1	F	151	GLN
1	F	159	SER
1	F	182	LEU
1	F	197	VAL
1	F	201	ARG
1	F	208	THR
1	F	218	LYS
1	F	224	LYS
1	F	225	LYS
1	F	237	THR
1	F	247	ARG
1	F	257	SER
1	F	258	VAL
1	F	260	THR
1	F	275	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	41	ASN
1	A	57	ASN
1	A	151	GLN

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Mol	Chain	Res	Type
1	A	192	ASN
1	A	262	GLN
1	A	266	HIS
1	A	278	GLN
1	A	279	HIS
1	B	35	GLN
1	B	57	ASN
1	B	91	ASN
1	B	156	ASN
1	B	192	ASN
1	B	279	HIS
1	C	41	ASN
1	C	91	ASN
1	C	100	HIS
1	C	142	ASN
1	C	199	ASN
1	C	250	GLN
1	C	266	HIS
1	C	278	GLN
1	C	279	HIS
1	D	6	ASN
1	D	70	GLN
1	D	100	HIS
1	D	142	ASN
1	D	229	HIS
1	D	242	ASN
1	D	250	GLN
1	D	262	GLN
1	D	266	HIS
1	D	279	HIS
1	E	70	GLN
1	E	91	ASN
1	E	192	ASN
1	E	199	ASN
1	E	262	GLN
1	E	279	HIS
1	F	91	ASN
1	F	142	ASN
1	F	151	GLN
1	F	199	ASN
1	F	242	ASN
1	F	279	HIS

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

15 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	$\#\|Z\| > 2$
2	PO4	A	301	-	4,4,4	0.31	0	6,6,6	0.25	0
2	PO4	A	302	-	4,4,4	0.46	0	6,6,6	0.28	0
2	PO4	A	303	-	4,4,4	0.41	0	6,6,6	0.26	0
2	PO4	A	304	-	4,4,4	0.45	0	6,6,6	0.22	0
2	PO4	B	301	-	4,4,4	0.57	0	6,6,6	0.23	0
2	PO4	B	302	-	4,4,4	0.43	0	6,6,6	0.25	0
2	PO4	C	301	-	4,4,4	0.62	0	6,6,6	0.26	0
2	PO4	C	302	-	4,4,4	0.41	0	6,6,6	0.29	0
2	PO4	C	303	-	4,4,4	0.12	0	6,6,6	0.24	0
2	PO4	D	301	-	4,4,4	0.52	0	6,6,6	0.28	0
2	PO4	D	302	-	4,4,4	0.38	0	6,6,6	0.29	0
2	PO4	E	301	-	4,4,4	0.43	0	6,6,6	0.25	0
2	PO4	E	302	-	4,4,4	0.45	0	6,6,6	0.30	0
2	PO4	F	301	-	4,4,4	0.35	0	6,6,6	0.27	0
2	PO4	F	302	-	4,4,4	0.38	0	6,6,6	0.25	0

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
2	PO4	A	301	-	-	0/0/0/0	0/0/0/0
2	PO4	A	302	-	-	0/0/0/0	0/0/0/0
2	PO4	A	303	-	-	0/0/0/0	0/0/0/0
2	PO4	A	304	-	-	0/0/0/0	0/0/0/0
2	PO4	B	301	-	-	0/0/0/0	0/0/0/0
2	PO4	B	302	-	-	0/0/0/0	0/0/0/0
2	PO4	C	301	-	-	0/0/0/0	0/0/0/0
2	PO4	C	302	-	-	0/0/0/0	0/0/0/0
2	PO4	C	303	-	-	0/0/0/0	0/0/0/0
2	PO4	D	301	-	-	0/0/0/0	0/0/0/0
2	PO4	D	302	-	-	0/0/0/0	0/0/0/0
2	PO4	E	301	-	-	0/0/0/0	0/0/0/0
2	PO4	E	302	-	-	0/0/0/0	0/0/0/0
2	PO4	F	301	-	-	0/0/0/0	0/0/0/0
2	PO4	F	302	-	-	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.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PO4	3	0
2	A	302	PO4	1	0
2	A	304	PO4	2	0
2	B	301	PO4	3	0
2	B	302	PO4	1	0
2	C	301	PO4	1	0
2	C	303	PO4	2	0
2	D	301	PO4	2	0
2	D	302	PO4	1	0
2	E	302	PO4	1	0

5.7 Other polymers

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

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, 95^{th} 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	271/317 (85%)	-0.31	2 (0%)	89	90	19, 33, 63, 87	0
1	B	266/317 (83%)	-0.40	1 (0%)	93	93	15, 25, 51, 80	0
1	C	268/317 (84%)	-0.37	6 (2%)	65	69	14, 24, 50, 87	0
1	D	265/317 (83%)	-0.21	2 (0%)	87	89	21, 34, 63, 83	0
1	E	271/317 (85%)	-0.36	3 (1%)	82	84	14, 25, 54, 89	0
1	F	259/317 (81%)	-0.21	3 (1%)	81	83	21, 36, 60, 83	0
All	All	1600/1902 (84%)	-0.31	17 (1%)	82	84	14, 30, 60, 89	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	160	GLY	5.5
1	C	99	SER	3.6
1	C	98	PRO	3.2
1	F	20	ARG	3.2
1	A	20	ARG	2.9
1	F	159	SER	2.8
1	E	161	LYS	2.7
1	C	96	LYS	2.5
1	F	160	GLY	2.4
1	D	20	ARG	2.3
1	E	99	SER	2.3
1	B	99	SER	2.3
1	C	100	HIS	2.3
1	D	95	PRO	2.2
1	E	100	HIS	2.2
1	C	4	GLU	2.2
1	C	95	PRO	2.0

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. 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, 95^{th} 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(Å^2)	Q<0.9
2	PO4	D	301	5/5	0.93	0.24	5.78	77,77,81,82	0
2	PO4	C	302	5/5	0.94	0.23	4.73	43,46,49,49	0
2	PO4	B	301	5/5	0.91	0.19	3.70	54,57,61,62	0
2	PO4	F	302	5/5	0.90	0.19	3.66	69,74,78,79	0
2	PO4	A	302	5/5	0.93	0.25	2.42	54,56,62,63	0
2	PO4	A	304	5/5	0.84	0.25	1.98	70,74,84,84	0
2	PO4	E	302	5/5	0.93	0.17	1.94	45,46,47,55	0
2	PO4	C	301	5/5	0.95	0.15	1.37	45,49,52,56	0
2	PO4	A	301	5/5	0.95	0.12	-1.66	59,61,68,69	0
2	PO4	F	301	5/5	0.92	0.17	-	56,57,65,69	0
2	PO4	E	301	5/5	0.94	0.17	-	50,53,60,62	0
2	PO4	A	303	5/5	0.89	0.18	-	65,74,82,84	0
2	PO4	B	302	5/5	0.91	0.24	-	59,64,68,68	0
2	PO4	D	302	5/5	0.89	0.25	-	54,62,67,69	0
2	PO4	C	303	5/5	0.89	0.32	-	43,55,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.