



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 04:29 am BST

PDB ID : 1OK4  
Title : Archaeal fructose 1,6-bisphosphate aldolase covalently bound to the substrate dihydroxyacetone phosphate  
Authors : Lorentzen, E.; Zwart, P.; Stark, A.; Hensel, R.; Siebers, B.; Pohl, E.  
Deposited on : 2003-07-17  
Resolution : 2.10 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](mailto: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.

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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

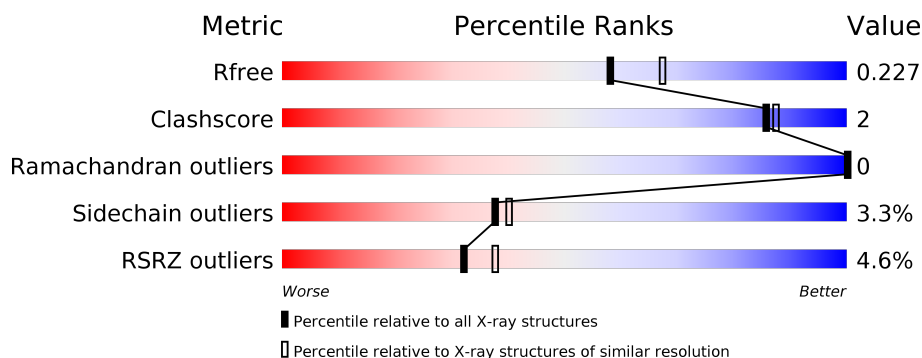
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	A	263	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	263	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	C	263	<div> <div>8%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>5%</div> </div> </div>
1	D	263	<div> <div>11%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>5%</div> </div> </div>
1	E	263	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>•</div> </div> </div>
1	F	263	<div> <div>8%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	263	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>%</div><div>89%</div><div>7%</div><div>5%</div></div>
1	H	263	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>85%</div><div>10%</div><div>5%</div></div>
1	I	263	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>89%</div><div>6%</div><div>5%</div></div>
1	J	263	<div><div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div><div>2%</div><div>87%</div><div>8%</div><div>5%</div></div>

## 2 Entry composition

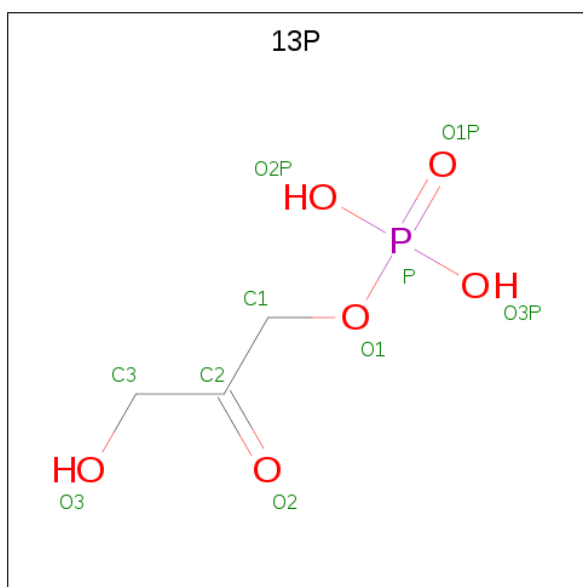
There are 3 unique types of molecules in this entry. The entry contains 20089 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	B	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	C	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	D	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	E	253	Total 1943	C 1251	N 331	O 356	S 5	0	0	1
1	F	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	G	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	H	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	I	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1
1	J	251	Total 1935	C 1247	N 329	O 354	S 5	0	0	1

- Molecule 2 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	66	Total	O	0	0
			66	66		

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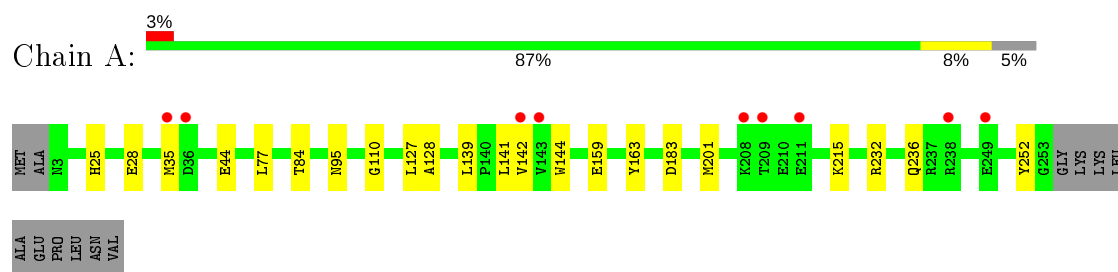
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	56	Total 56	O 56	0	0
3	D	53	Total 53	O 53	0	0
3	E	63	Total 63	O 63	0	0
3	F	51	Total 51	O 51	0	0
3	G	76	Total 76	O 76	0	0
3	H	68	Total 68	O 68	0	0
3	I	71	Total 71	O 71	0	0
3	J	65	Total 65	O 65	0	0

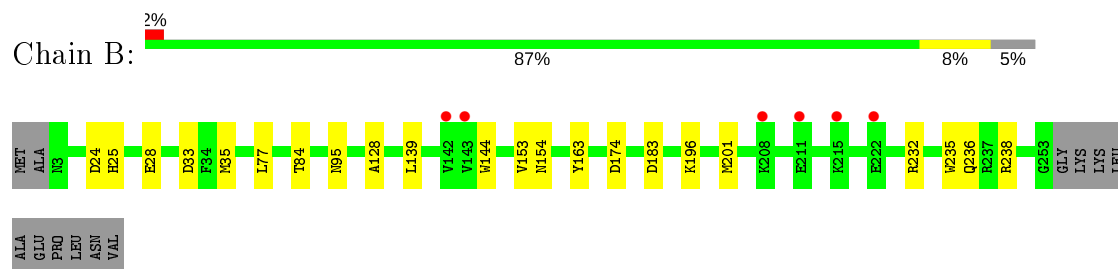
### 3 Residue-property plots [i](#)

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.

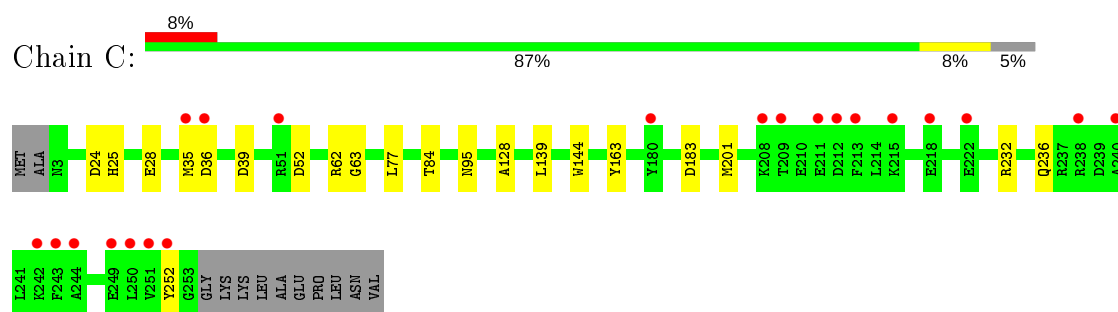
#### • Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



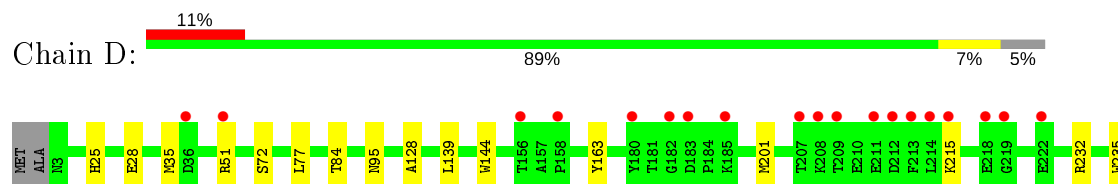
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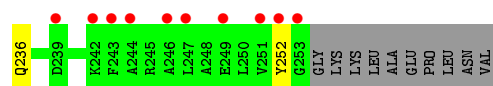


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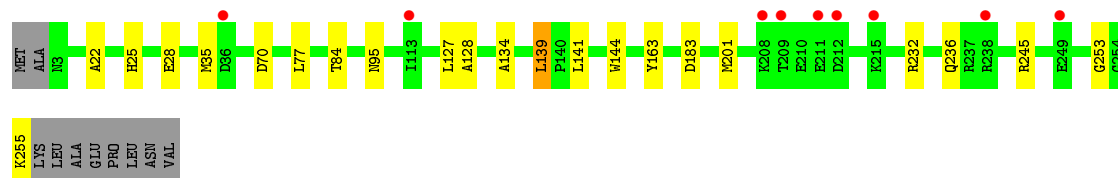
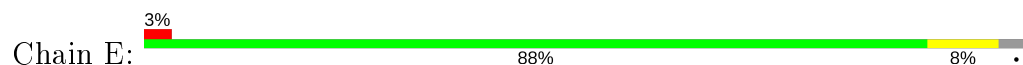


#### • Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

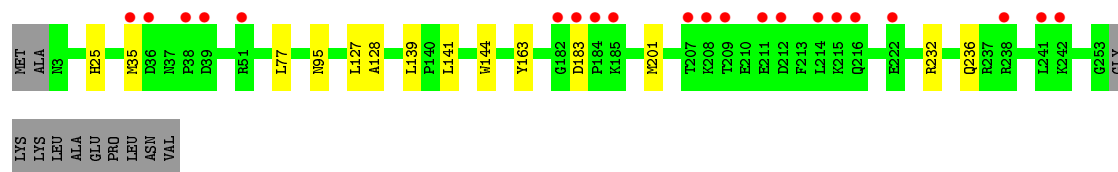
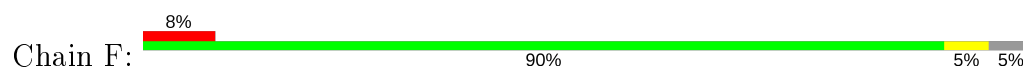




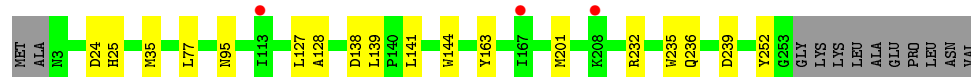
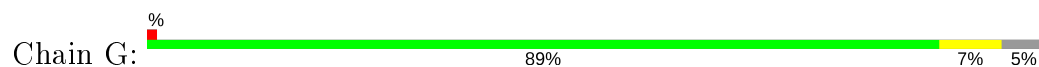
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



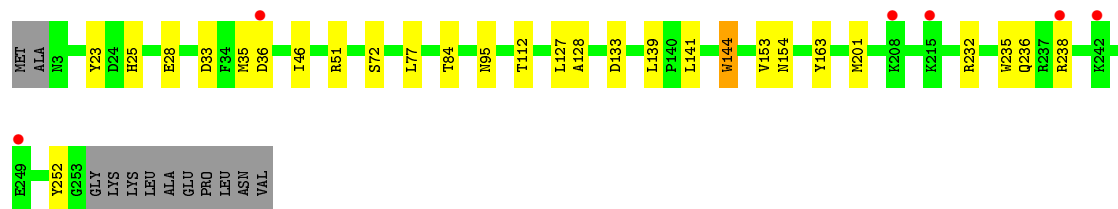
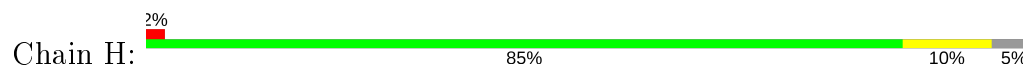
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



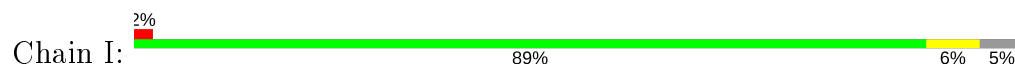
• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

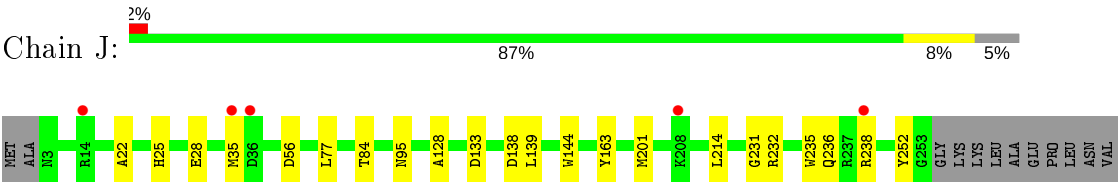


• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.40Å 157.30Å 101.50Å 90.00° 108.20° 90.00°	Depositor
Resolution (Å)	36.51 – 2.10 36.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.51-2.10) 90.2 (36.41-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.163 , 0.185 0.207 , 0.227	Depositor DCC
$R_{free}$ test set	3203 reflections (2.49%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.9	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 13P

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	0.62	1/1978 (0.1%)	0.76	1/2678 (0.0%)
1	B	0.68	0/1978	0.78	6/2678 (0.2%)
1	C	0.60	1/1978 (0.1%)	0.76	5/2678 (0.2%)
1	D	0.56	1/1978 (0.1%)	0.76	0/2678
1	E	0.64	0/1986	0.78	2/2688 (0.1%)
1	F	0.62	0/1978	0.77	1/2678 (0.0%)
1	G	0.66	1/1978 (0.1%)	0.77	2/2678 (0.1%)
1	H	0.65	1/1978 (0.1%)	0.78	3/2678 (0.1%)
1	I	0.63	1/1978 (0.1%)	0.76	2/2678 (0.1%)
1	J	0.69	1/1978 (0.1%)	0.79	3/2678 (0.1%)
All	All	0.64	7/19788 (0.0%)	0.77	25/26790 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	TYR	C-N	-6.72	1.21	1.33
1	G	252	TYR	C-N	-6.26	1.21	1.33
1	I	252	TYR	C-N	-6.24	1.21	1.33
1	H	252	TYR	C-N	-6.16	1.22	1.33
1	J	252	TYR	C-N	-5.98	1.22	1.33
1	D	252	TYR	C-N	-5.58	1.23	1.33
1	A	252	TYR	C-N	-5.25	1.23	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	133	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	183	ASP	CB-CG-OD2	6.06	123.76	118.30
1	B	183	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	238	ARG	NE-CZ-NH1	5.65	123.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	138	ASP	CB-CG-OD2	5.63	123.37	118.30
1	I	24	ASP	CB-CG-OD2	5.63	123.37	118.30
1	I	183	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	183	ASP	CB-CG-OD2	5.55	123.30	118.30
1	J	56	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	36	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	24	ASP	CB-CG-OD2	5.48	123.24	118.30
1	B	174	ASP	CB-CG-OD2	5.43	123.19	118.30
1	E	183	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	238	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	70	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	24	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	52	ASP	CB-CG-OD2	5.24	123.01	118.30
1	G	24	ASP	CB-CG-OD2	5.23	123.00	118.30
1	J	138	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	33	ASP	CB-CG-OD2	5.18	122.97	118.30
1	H	33	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	39	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	183	ASP	CB-CG-OD2	5.06	122.86	118.30
1	H	133	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	36	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1935	0	1946	10	0
1	B	1935	0	1947	13	0
1	C	1935	0	1946	6	0
1	D	1935	0	1946	7	0
1	E	1943	0	1952	10	0
1	F	1935	0	1946	5	0
1	G	1935	0	1946	8	0
1	H	1935	0	1946	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1935	0	1946	7	0
1	J	1935	0	1946	11	0
2	A	9	0	5	2	0
2	B	9	0	5	0	0
2	C	9	0	5	1	0
2	D	9	0	5	0	0
2	E	9	0	5	3	0
2	F	9	0	5	2	0
2	G	9	0	5	0	0
2	H	9	0	5	0	0
2	I	9	0	5	1	0
2	J	9	0	5	3	0
3	A	72	0	0	3	0
3	B	66	0	0	0	0
3	C	56	0	0	0	0
3	D	53	0	0	0	0
3	E	63	0	0	0	0
3	F	51	0	0	1	0
3	G	76	0	0	1	0
3	H	68	0	0	0	0
3	I	71	0	0	1	0
3	J	65	0	0	1	0
All	All	20089	0	19517	86	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 2.

All (86) 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:159:GLU:OE1	3:A:2056:HOH:O	1.59	1.18
1:H:25:HIS:CD2	1:H:235:TRP:HZ2	1.71	1.09
1:J:25:HIS:ND1	1:J:235:TRP:HZ2	1.60	1.00
1:H:25:HIS:HD2	1:H:235:TRP:CZ2	1.82	0.98
1:H:25:HIS:CD2	1:H:235:TRP:CZ2	2.53	0.97
1:B:25:HIS:HD2	1:B:235:TRP:CZ2	1.83	0.96
1:B:25:HIS:CD2	1:B:235:TRP:HZ2	1.84	0.94
1:B:25:HIS:HD2	1:B:235:TRP:HZ2	0.96	0.92
1:I:25:HIS:CD2	1:I:235:TRP:HZ2	1.88	0.91
1:G:25:HIS:HD1	1:G:235:TRP:HZ2	1.17	0.86
1:G:239:ASP:OD2	3:G:2073:HOH:O	1.94	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:25:HIS:ND1	1:G:235:TRP:HZ2	1.78	0.81
1:A:25:HIS:HE1	2:A:1254:13P:O2P	1.63	0.81
1:J:25:HIS:ND1	1:J:235:TRP:CZ2	2.43	0.80
1:B:25:HIS:CD2	1:B:235:TRP:CZ2	2.67	0.75
1:I:25:HIS:HD2	1:I:235:TRP:HZ2	1.34	0.75
1:J:25:HIS:HD1	1:J:235:TRP:HZ2	0.82	0.70
1:I:25:HIS:CD2	1:I:235:TRP:CZ2	2.79	0.68
1:E:25:HIS:HE1	2:E:1256:13P:O2P	1.77	0.66
1:H:153:VAL:HG23	1:H:154:ASN:H	1.61	0.65
1:C:25:HIS:HE1	2:C:1254:13P:O2P	1.81	0.63
1:F:25:HIS:HE1	2:F:1254:13P:O2P	1.81	0.63
1:A:25:HIS:CE1	2:A:1254:13P:O2P	2.49	0.63
3:A:2015:HOH:O	1:B:196:LYS:NZ	2.21	0.60
1:B:153:VAL:HG23	1:B:154:ASN:N	2.22	0.55
1:D:25:HIS:CD2	1:D:235:TRP:HZ2	2.25	0.55
2:I:1254:13P:C2	3:I:2070:HOH:O	2.56	0.53
1:H:23:TYR:CE1	1:H:46:ILE:HG13	2.44	0.53
1:J:22:ALA:HB1	2:J:1254:13P:H32	1.91	0.53
1:A:44:GLU:OE1	3:A:2015:HOH:O	2.19	0.51
1:H:128:ALA:HB2	1:I:95:ASN:HA	1.91	0.51
1:F:232:ARG:O	1:F:236:GLN:HB2	2.10	0.51
1:J:25:HIS:HE1	1:J:231:GLY:HA3	1.76	0.51
1:H:232:ARG:O	1:H:236:GLN:HB2	2.11	0.51
1:A:232:ARG:O	1:A:236:GLN:HB2	2.10	0.50
1:E:232:ARG:O	1:E:236:GLN:HB2	2.11	0.50
1:H:51:ARG:HD2	1:H:72:SER:HB2	1.94	0.50
1:D:51:ARG:HD3	1:D:72:SER:HB2	1.94	0.50
1:C:95:ASN:HA	1:D:128:ALA:HB2	1.94	0.49
1:I:232:ARG:O	1:I:236:GLN:HB2	2.12	0.49
1:G:25:HIS:ND1	1:G:235:TRP:CZ2	2.69	0.49
1:J:232:ARG:O	1:J:236:GLN:HB2	2.11	0.49
1:C:232:ARG:O	1:C:236:GLN:HB2	2.12	0.49
1:G:232:ARG:O	1:G:236:GLN:HB2	2.12	0.49
1:H:28:GLU:O	1:H:84:THR:HG23	2.13	0.49
1:D:232:ARG:O	1:D:236:GLN:HB2	2.13	0.49
1:H:25:HIS:HD2	1:H:235:TRP:CH2	2.29	0.48
1:E:22:ALA:HB1	2:E:1256:13P:H32	1.95	0.48
1:D:95:ASN:HA	1:E:128:ALA:HB2	1.97	0.47
1:B:153:VAL:HG23	1:B:154:ASN:H	1.80	0.46
1:B:232:ARG:O	1:B:236:GLN:HB2	2.16	0.45
1:E:28:GLU:O	1:E:84:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:128:ALA:HB2	1:J:95:ASN:HA	1.98	0.45
1:A:95:ASN:HA	1:B:128:ALA:HB2	1.99	0.45
1:G:128:ALA:HB2	1:H:95:ASN:HA	1.99	0.44
1:F:95:ASN:HA	1:J:128:ALA:HB2	2.00	0.44
1:H:153:VAL:HG23	1:H:154:ASN:N	2.29	0.44
1:B:95:ASN:HA	1:C:128:ALA:HB2	1.99	0.43
2:J:1254:13P:C2	3:J:2065:HOH:O	2.67	0.43
1:E:25:HIS:CE1	2:E:1256:13P:O2P	2.65	0.43
1:D:28:GLU:O	1:D:84:THR:HG23	2.19	0.43
1:C:28:GLU:O	1:C:84:THR:HG23	2.19	0.42
1:G:127:LEU:HD11	1:G:141:LEU:HD21	2.01	0.42
1:H:127:LEU:HD11	1:H:141:LEU:HD21	2.02	0.42
1:J:28:GLU:O	1:J:84:THR:HG23	2.19	0.42
2:F:1254:13P:C2	3:F:2051:HOH:O	2.67	0.42
1:A:110:GLY:HA2	1:A:142:VAL:O	2.20	0.41
1:A:28:GLU:O	1:A:84:THR:HG23	2.19	0.41
1:B:153:VAL:CG2	1:B:154:ASN:N	2.82	0.41
1:F:127:LEU:HD11	1:F:141:LEU:HD21	2.02	0.41
1:E:253:GLY:O	1:E:255:LYS:N	2.53	0.41
1:H:23:TYR:CZ	1:H:46:ILE:HG13	2.55	0.41
1:B:153:VAL:CG2	1:B:154:ASN:H	2.33	0.41
1:J:214:LEU:HD23	1:J:214:LEU:HA	1.97	0.41
1:A:127:LEU:HD11	1:A:141:LEU:HD21	2.02	0.41
1:B:28:GLU:O	1:B:84:THR:HG23	2.21	0.41
1:E:127:LEU:HD11	1:E:141:LEU:HD21	2.02	0.41
1:A:128:ALA:HB2	1:E:95:ASN:HA	2.02	0.41
1:H:25:HIS:ND1	1:H:25:HIS:N	2.69	0.40
1:J:25:HIS:CE1	2:J:1254:13P:O2P	2.74	0.40
1:F:128:ALA:HB2	1:G:95:ASN:HA	2.03	0.40
1:I:110:GLY:HA2	1:I:142:VAL:O	2.21	0.40
1:E:134:ALA:HB1	1:E:139:LEU:O	2.22	0.40
1:H:112:THR:HA	1:H:144:TRP:HB2	2.03	0.40
1:C:62:ARG:HG3	1:C:63:GLY:N	2.36	0.40
1:D:51:ARG:CD	1:D:72:SER:HB2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	B	249/263 (95%)	243 (98%)	6 (2%)	0	100	100
1	C	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	D	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	E	251/263 (95%)	244 (97%)	7 (3%)	0	100	100
1	F	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	G	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	H	249/263 (95%)	243 (98%)	6 (2%)	0	100	100
1	I	249/263 (95%)	243 (98%)	6 (2%)	0	100	100
1	J	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
All	All	2492/2630 (95%)	2437 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/206 (96%)	190 (96%)	7 (4%)	35	36
1	B	197/206 (96%)	191 (97%)	6 (3%)	41	44
1	C	197/206 (96%)	191 (97%)	6 (3%)	41	44
1	D	197/206 (96%)	190 (96%)	7 (4%)	35	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	197/206 (96%)	190 (96%)	7 (4%)	35	36
1	F	197/206 (96%)	191 (97%)	6 (3%)	41	44
1	G	197/206 (96%)	191 (97%)	6 (3%)	41	44
1	H	197/206 (96%)	190 (96%)	7 (4%)	35	36
1	I	197/206 (96%)	191 (97%)	6 (3%)	41	44
1	J	197/206 (96%)	190 (96%)	7 (4%)	35	36
All	All	1970/2060 (96%)	1905 (97%)	65 (3%)	38	40

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	77	LEU
1	A	139	LEU
1	A	144	TRP
1	A	163	TYR
1	A	201	MET
1	A	215	LYS
1	B	35	MET
1	B	77	LEU
1	B	139	LEU
1	B	144	TRP
1	B	163	TYR
1	B	201	MET
1	C	35	MET
1	C	77	LEU
1	C	139	LEU
1	C	144	TRP
1	C	163	TYR
1	C	201	MET
1	D	35	MET
1	D	77	LEU
1	D	139	LEU
1	D	144	TRP
1	D	163	TYR
1	D	201	MET
1	D	215	LYS
1	E	35	MET
1	E	77	LEU
1	E	139	LEU

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Mol	Chain	Res	Type
1	E	144	TRP
1	E	163	TYR
1	E	201	MET
1	E	245	ARG
1	F	35	MET
1	F	77	LEU
1	F	139	LEU
1	F	144	TRP
1	F	163	TYR
1	F	201	MET
1	G	35	MET
1	G	77	LEU
1	G	139	LEU
1	G	144	TRP
1	G	163	TYR
1	G	201	MET
1	H	35	MET
1	H	77	LEU
1	H	139	LEU
1	H	144	TRP
1	H	163	TYR
1	H	201	MET
1	H	238	ARG
1	I	35	MET
1	I	77	LEU
1	I	139	LEU
1	I	144	TRP
1	I	163	TYR
1	I	201	MET
1	J	35	MET
1	J	77	LEU
1	J	139	LEU
1	J	144	TRP
1	J	163	TYR
1	J	201	MET
1	J	238	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	B	25	HIS

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Mol	Chain	Res	Type
1	C	25	HIS
1	D	25	HIS
1	E	25	HIS
1	E	29	HIS
1	F	25	HIS
1	H	25	HIS
1	I	25	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

10 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	13P	C	1254	1	8,8,9	1.02	1 (12%)	10,10,12	1.31	1 (10%)
2	13P	F	1254	1	8,8,9	0.95	1 (12%)	10,10,12	1.47	1 (10%)
2	13P	G	1254	1	8,8,9	1.02	1 (12%)	10,10,12	1.35	1 (10%)
2	13P	D	1254	1	8,8,9	1.19	1 (12%)	10,10,12	0.89	0
2	13P	E	1256	1	8,8,9	1.07	1 (12%)	10,10,12	1.78	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	13P	I	1254	1	8,8,9	0.99	1 (12%)	10,10,12	1.41	1 (10%)
2	13P	J	1254	1	8,8,9	0.89	0	10,10,12	0.97	0
2	13P	H	1254	1	8,8,9	1.15	1 (12%)	10,10,12	1.81	2 (20%)
2	13P	A	1254	1	8,8,9	1.04	1 (12%)	10,10,12	1.78	2 (20%)
2	13P	B	1254	1	8,8,9	0.96	0	10,10,12	1.70	1 (10%)

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	13P	C	1254	1	-	2/6/6/8	-
2	13P	F	1254	1	-	1/6/6/8	-
2	13P	G	1254	1	-	1/6/6/8	-
2	13P	D	1254	1	-	1/6/6/8	-
2	13P	E	1256	1	-	2/6/6/8	-
2	13P	I	1254	1	-	1/6/6/8	-
2	13P	J	1254	1	-	1/6/6/8	-
2	13P	H	1254	1	-	2/6/6/8	-
2	13P	A	1254	1	-	2/6/6/8	-
2	13P	B	1254	1	-	2/6/6/8	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1254	13P	P-O1P	2.77	1.59	1.50
2	H	1254	13P	P-O1P	2.65	1.59	1.50
2	C	1254	13P	P-O1P	2.49	1.58	1.50
2	A	1254	13P	P-O1P	2.35	1.58	1.50
2	I	1254	13P	P-O1P	2.34	1.58	1.50
2	E	1256	13P	P-O1P	2.34	1.58	1.50
2	F	1254	13P	P-O1P	2.23	1.57	1.50
2	G	1254	13P	P-O1P	2.14	1.57	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1254	13P	C1-C2-C3	4.63	124.05	113.95
2	A	1254	13P	C1-C2-C3	4.36	123.45	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1254	13P	C1-C2-C3	4.31	123.35	113.95
2	E	1256	13P	C1-C2-C3	3.78	122.18	113.95
2	F	1254	13P	C1-C2-C3	3.77	122.17	113.95
2	I	1254	13P	C1-C2-C3	3.35	121.26	113.95
2	G	1254	13P	C1-C2-C3	3.08	120.67	113.95
2	C	1254	13P	C1-C2-C3	2.72	119.87	113.95
2	E	1256	13P	O1-P-O1P	2.65	113.92	106.47
2	A	1254	13P	O3P-P-O1	2.63	113.72	106.73
2	H	1254	13P	O2P-P-O1	2.48	113.33	106.73

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1254	13P	C1-C2-C3-O3
2	G	1254	13P	C1-C2-C3-O3
2	I	1254	13P	C1-C2-C3-O3
2	J	1254	13P	C1-C2-C3-O3
2	H	1254	13P	C1-C2-C3-O3
2	A	1254	13P	C1-C2-C3-O3
2	B	1254	13P	C1-C2-C3-O3
2	H	1254	13P	O1-C1-C2-C3
2	D	1254	13P	O1-C1-C2-C3
2	E	1256	13P	C1-C2-C3-O3
2	B	1254	13P	O1-C1-C2-C3
2	F	1254	13P	O1-C1-C2-C3
2	A	1254	13P	O1-C1-C2-C3
2	C	1254	13P	O1-C1-C2-C3
2	E	1256	13P	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1254	13P	1	0
2	F	1254	13P	2	0
2	E	1256	13P	3	0
2	I	1254	13P	1	0
2	J	1254	13P	3	0
2	A	1254	13P	2	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	251/263 (95%)	0.29	9 (3%)	42 49	4, 9, 18, 26	0
1	B	251/263 (95%)	0.26	6 (2%)	59 64	4, 8, 18, 26	0
1	C	251/263 (95%)	0.43	21 (8%)	11 14	4, 9, 18, 26	0
1	D	251/263 (95%)	0.43	29 (11%)	4 6	4, 9, 18, 26	0
1	E	253/263 (96%)	0.20	9 (3%)	42 49	4, 9, 18, 26	0
1	F	251/263 (95%)	0.39	21 (8%)	11 14	4, 9, 18, 26	0
1	G	251/263 (95%)	0.14	3 (1%)	79 82	4, 9, 18, 26	0
1	H	251/263 (95%)	0.28	6 (2%)	59 64	4, 9, 18, 26	0
1	I	251/263 (95%)	0.22	6 (2%)	59 64	4, 9, 18, 26	0
1	J	251/263 (95%)	0.09	5 (1%)	65 69	4, 8, 18, 26	0
All	All	2512/2630 (95%)	0.27	115 (4%)	32 38	4, 9, 18, 26	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	208	LYS	4.9
1	C	249	GLU	4.2
1	C	35	MET	4.1
1	D	211	GLU	4.0
1	J	208	LYS	3.9
1	D	209	THR	3.8
1	A	238	ARG	3.8
1	D	242	LYS	3.8
1	D	214	LEU	3.8
1	C	218	GLU	3.7
1	B	208	LYS	3.6
1	F	215	LYS	3.6
1	D	185	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	212	ASP	3.6
1	D	247	LEU	3.4
1	E	238	ARG	3.4
1	C	238	ARG	3.4
1	F	182	GLY	3.4
1	A	35	MET	3.3
1	F	35	MET	3.3
1	C	208	LYS	3.3
1	D	215	LYS	3.3
1	J	35	MET	3.3
1	F	212	ASP	3.2
1	A	249	GLU	3.2
1	F	36	ASP	3.2
1	D	249	GLU	3.1
1	F	51	ARG	3.1
1	C	211	GLU	3.1
1	D	213	PHE	3.1
1	D	243	PHE	3.1
1	A	208	LYS	3.0
1	C	240	ALA	2.9
1	D	180	TYR	2.9
1	E	208	LYS	2.9
1	F	222	GLU	2.9
1	J	238	ARG	2.9
1	F	211	GLU	2.9
1	D	218	GLU	2.9
1	E	36	ASP	2.8
1	F	209	THR	2.8
1	D	246	ALA	2.8
1	D	222	GLU	2.8
1	F	238	ARG	2.8
1	D	36	ASP	2.8
1	C	251	VAL	2.7
1	C	250	LEU	2.7
1	C	222	GLU	2.7
1	H	238	ARG	2.7
1	C	242	LYS	2.6
1	C	243	PHE	2.6
1	D	219	GLY	2.6
1	H	36	ASP	2.6
1	C	213	PHE	2.6
1	C	36	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	249	GLU	2.6
1	A	142	VAL	2.6
1	C	252	TYR	2.6
1	H	249	GLU	2.6
1	D	182	GLY	2.5
1	G	208	LYS	2.5
1	F	214	LEU	2.5
1	G	167	ILE	2.5
1	C	244	ALA	2.5
1	D	183	ASP	2.5
1	D	251	VAL	2.5
1	F	184	PRO	2.5
1	A	36	ASP	2.5
1	B	222	GLU	2.5
1	H	208	LYS	2.5
1	C	209	THR	2.4
1	B	215	LYS	2.4
1	C	212	ASP	2.4
1	G	113	ILE	2.4
1	D	239	ASP	2.4
1	E	209	THR	2.4
1	B	211	GLU	2.3
1	F	183	ASP	2.3
1	D	252	TYR	2.3
1	F	207	THR	2.3
1	E	212	ASP	2.3
1	F	216	GLN	2.3
1	J	14	ARG	2.3
1	D	51	ARG	2.2
1	F	208	LYS	2.2
1	F	242	LYS	2.2
1	E	249	GLU	2.2
1	D	253	GLY	2.2
1	A	211	GLU	2.2
1	I	222	GLU	2.2
1	I	171	LEU	2.2
1	B	142	VAL	2.2
1	I	218	GLU	2.2
1	D	158	PRO	2.2
1	F	241	LEU	2.1
1	E	211	GLU	2.1
1	A	209	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	215	LYS	2.1
1	E	113	ILE	2.1
1	H	215	LYS	2.1
1	A	143	VAL	2.1
1	D	207	THR	2.1
1	J	36	ASP	2.1
1	I	212	ASP	2.1
1	D	244	ALA	2.1
1	C	180	TYR	2.1
1	C	215	LYS	2.1
1	F	185	LYS	2.1
1	C	51	ARG	2.0
1	F	38	PRO	2.0
1	H	242	LYS	2.0
1	I	215	LYS	2.0
1	D	156	THR	2.0
1	F	39	ASP	2.0
1	B	143	VAL	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
2	13P	C	1254	9/10	0.93	0.15	8,13,16,17	0
2	13P	F	1254	9/10	0.93	0.14	13,15,21,24	0
2	13P	G	1254	9/10	0.94	0.16	10,12,24,31	0
2	13P	E	1256	9/10	0.94	0.11	8,13,21,26	0
2	13P	H	1254	9/10	0.94	0.13	13,17,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	13P	A	1254	9/10	0.94	0.12	11,14,21,25	0
2	13P	D	1254	9/10	0.95	0.10	11,13,17,18	0
2	13P	B	1254	9/10	0.95	0.13	10,12,24,25	0
2	13P	J	1254	9/10	0.96	0.09	8,11,22,25	0
2	13P	I	1254	9/10	0.96	0.12	13,17,22,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.