



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:02 PM GMT

PDB ID : 1W8S
Title : THE MECHANISM OF THE SCHIFF BASE FORMING FRUCTOSE-1,6-BISPHOSPHATE ALDOLASE: STRUCTURAL ANALYSIS OF REACTION INTERMEDIATES
Authors : Lorentzen, E.; Hensel, R.; Siebers, B.; Pohl, E.
Deposited on : 2004-09-27
Resolution : 1.85 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

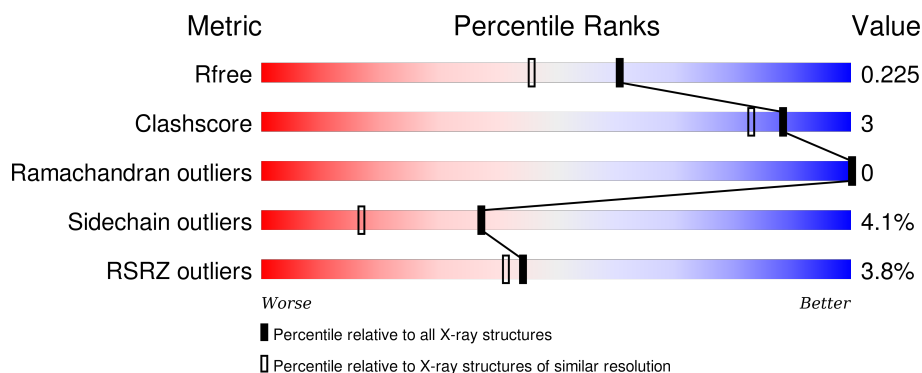
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	<div> <div>3%</div> <div>86% 9% 5%</div> </div>
1	B	263	<div> <div>3%</div> <div>87% 6% 5%</div> </div>
1	C	263	<div> <div>8%</div> <div>86% 9% 5%</div> </div>
1	D	263	<div> <div>4%</div> <div>86% 8% 5%</div> </div>
1	E	263	<div> <div>3%</div> <div>86% 9% .</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	263	<div><div></div><div>5%</div><div>87%</div><div>7%5%</div></div>
1	G	263	<div><div></div><div>2%</div><div>87%</div><div>8%5%</div></div>
1	H	263	<div><div></div><div>4%</div><div>83%</div><div>11%5%</div></div>
1	I	263	<div><div></div><div>3%</div><div>89%</div><div>6%5%</div></div>
1	J	263	<div><div></div><div>%</div><div>87%</div><div>8%5%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20960 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	250	Total	C	N	O	S	0	3	0
			1940	1248	327	359	6			
1	B	250	Total	C	N	O	S	0	1	0
			1931	1242	327	357	5			
1	C	250	Total	C	N	O	S	0	2	0
			1936	1246	328	357	5			
1	D	250	Total	C	N	O	S	0	1	0
			1936	1245	330	356	5			
1	E	252	Total	C	N	O	S	0	2	0
			1942	1248	329	359	6			
1	F	250	Total	C	N	O	S	0	2	0
			1937	1245	330	356	6			
1	G	250	Total	C	N	O	S	0	4	0
			1949	1253	330	360	6			
1	H	250	Total	C	N	O	S	0	4	0
			1947	1252	331	359	5			
1	I	250	Total	C	N	O	S	0	2	0
			1935	1245	327	357	6			
1	J	250	Total	C	N	O	S	0	4	0
			1945	1252	328	359	6			

There are 20 discrepancies between the modelled and reference sequences:

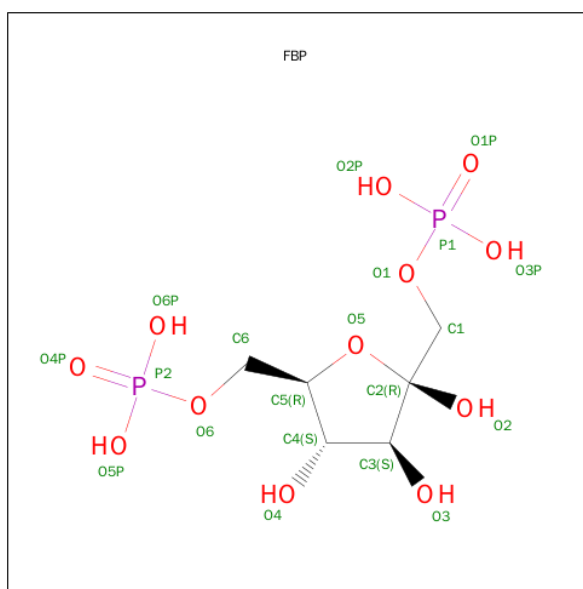
Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
B	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
C	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
D	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
E	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
F	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
G	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
H	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
I	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	144	GLU	TRP	ENGINEERED MUTATION	UNP P58315
A	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
B	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
C	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
D	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
E	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
F	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
G	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
H	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
I	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315
J	146	PHE	TYR	ENGINEERED MUTATION	UNP P58315

- Molecule 2 is SUGAR (BETA-FRUCTOSE-1,6-DIPHOSPHATE) (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		
2	E	1	Total	C	O	P	0	0
			20	6	12	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		
2	I	1	Total	C	O	P	0	0
			20	6	12	2		
2	J	1	Total	C	O	P	0	0
			20	6	12	2		

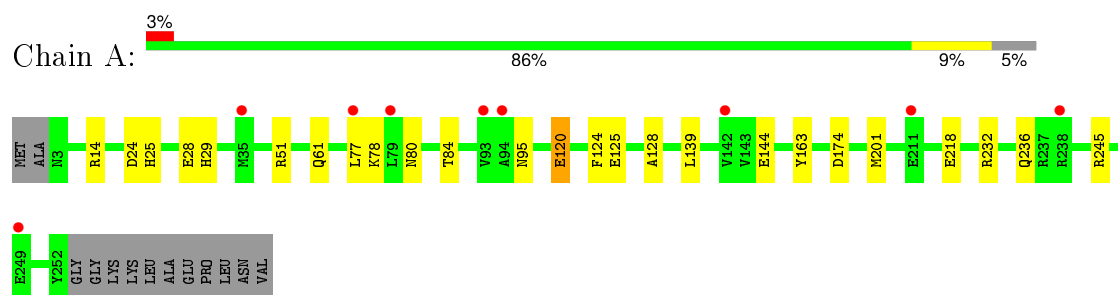
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total	O	0	0
			140	140		
3	B	154	Total	O	0	0
			154	154		
3	C	119	Total	O	0	0
			119	119		
3	D	111	Total	O	0	0
			111	111		
3	E	135	Total	O	0	0
			135	135		
3	F	115	Total	O	0	0
			115	115		
3	G	133	Total	O	0	0
			133	133		
3	H	147	Total	O	0	0
			147	147		
3	I	149	Total	O	0	0
			149	149		
3	J	159	Total	O	0	0
			159	159		

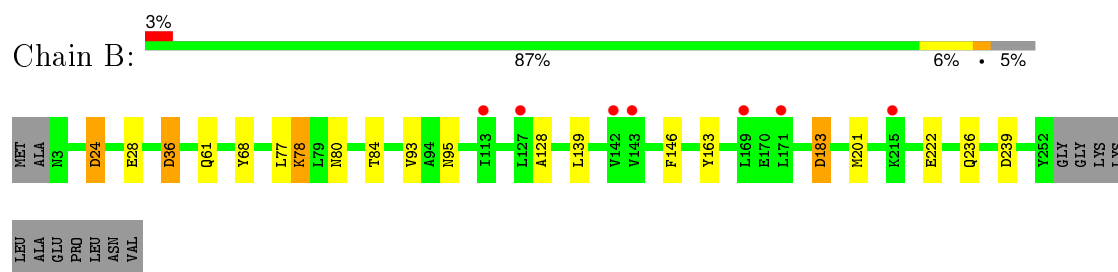
3 Residue-property plots [i](#)

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.

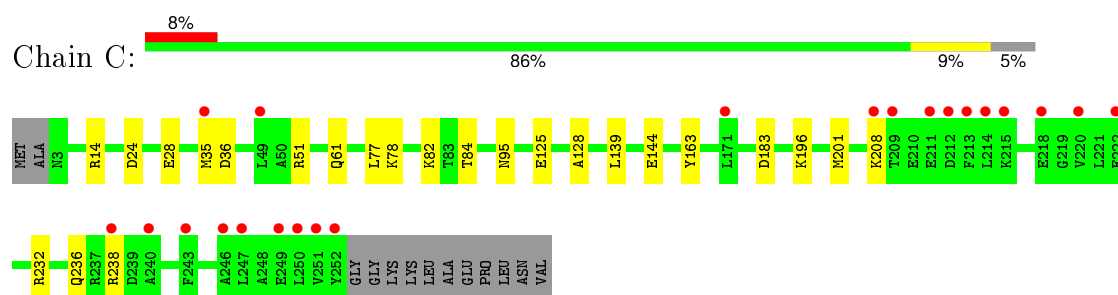
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



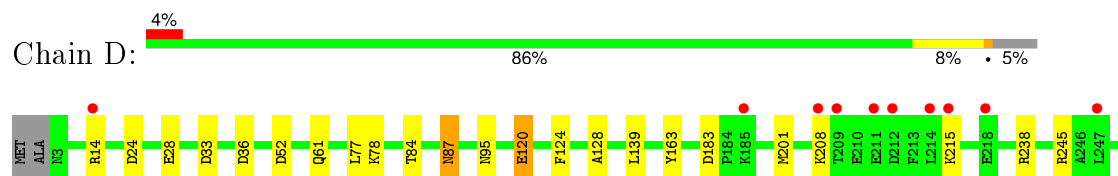
- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

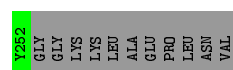


- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

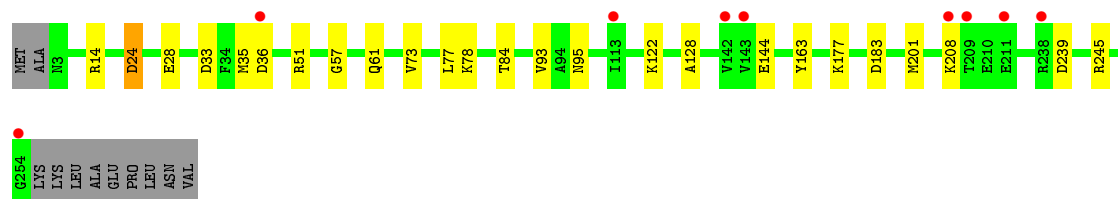
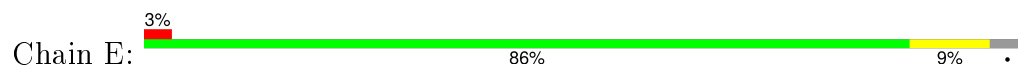


- Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I

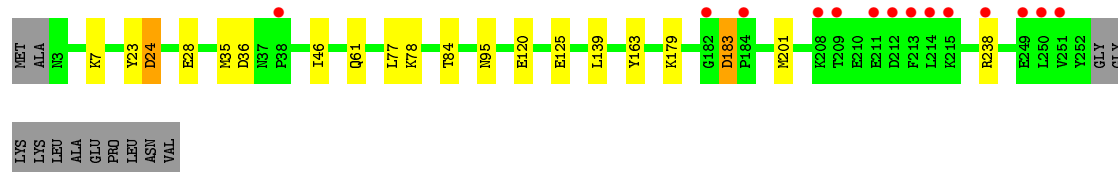
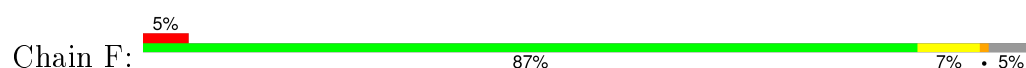




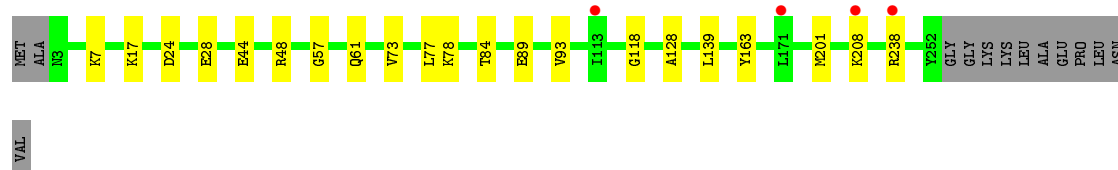
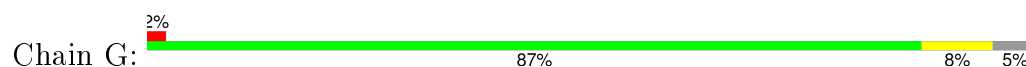
● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



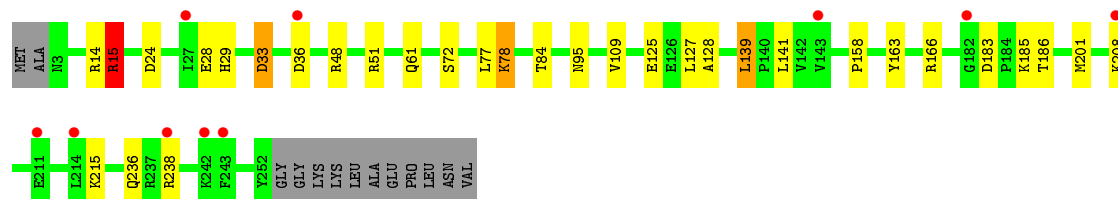
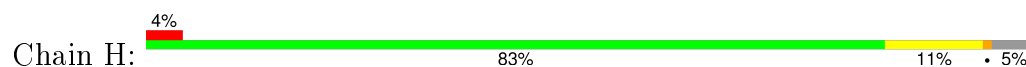
● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



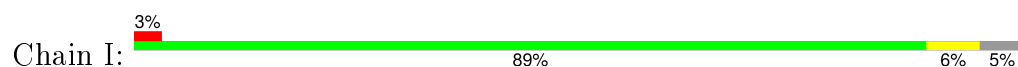
● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



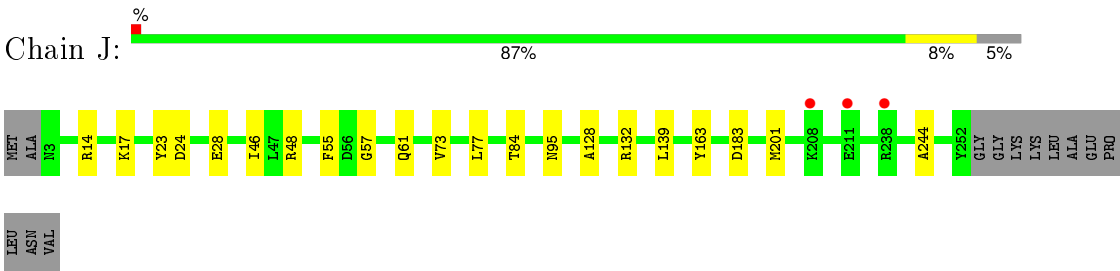
● Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE CLASS I



● 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, α , β , γ	82.50Å 157.30Å 101.20Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 37.39 – 1.85	Depositor EDS
% Data completeness (in resolution range)	1.0 (40.00-1.85) 95.6 (37.39-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.187 0.198 , 0.225	Depositor DCC
R_{free} test set	2016 reflections (1.01%)	DCC
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 199615 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20960	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.68	0/1993	0.81	1/2695 (0.0%)
1	B	0.70	0/1976	0.80	4/2673 (0.1%)
1	C	0.66	0/1985	0.82	2/2684 (0.1%)
1	D	0.68	1/1981 (0.1%)	0.82	3/2679 (0.1%)
1	E	0.67	0/1992	0.78	3/2693 (0.1%)
1	F	0.67	0/1989	0.78	3/2689 (0.1%)
1	G	0.71	0/2007	0.84	1/2714 (0.0%)
1	H	0.72	2/2004 (0.1%)	0.85	6/2709 (0.2%)
1	I	0.71	0/1984	0.79	1/2683 (0.0%)
1	J	0.70	0/2002	0.85	3/2706 (0.1%)
All	All	0.69	3/19913 (0.0%)	0.82	27/26925 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	78	LYS	CE-NZ	5.53	1.62	1.49
1	D	78	LYS	CD-CE	5.21	1.64	1.51
1	H	78	LYS	CD-CE	5.16	1.64	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	132	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	G	238	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	174	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	36	ASP	CB-CG-OD2	6.37	124.03	118.30
1	D	36	ASP	CB-CG-OD2	6.05	123.74	118.30
1	D	183	ASP	CB-CG-OD2	6.01	123.71	118.30
1	F	36	ASP	CB-CG-OD2	5.97	123.67	118.30
1	H	36	ASP	CB-CG-OD2	5.95	123.66	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	33[A]	ASP	CB-CG-OD2	5.91	123.61	118.30
1	H	33[B]	ASP	CB-CG-OD2	5.91	123.61	118.30
1	F	24	ASP	CB-CG-OD2	5.82	123.54	118.30
1	I	183	ASP	CB-CG-OD2	5.73	123.46	118.30
1	H	15	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	183	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	24	ASP	CB-CG-OD2	5.40	123.16	118.30
1	J	183	ASP	CB-CG-OD2	5.38	123.15	118.30
1	E	239	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	183	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	183	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	183	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	24	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	36	ASP	CB-CG-OD2	5.24	123.02	118.30
1	H	166	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	239	ASP	CB-CG-OD2	5.14	122.92	118.30
1	J	132	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	E	36	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	52	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	1940	0	1953	15	0
1	B	1931	0	1946	9	0
1	C	1936	0	1955	10	1
1	D	1936	0	1954	7	0
1	E	1942	0	1957	14	0
1	F	1937	0	1955	7	0
1	G	1949	0	1963	9	1
1	H	1947	0	1964	26	0
1	I	1935	0	1951	8	0
1	J	1945	0	1962	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	10	2	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
2	E	20	0	10	1	0
2	F	20	0	10	0	0
2	G	20	0	10	0	0
2	H	20	0	10	1	0
2	I	20	0	10	1	0
2	J	20	0	10	0	0
3	A	140	0	0	1	0
3	B	154	0	0	1	0
3	C	119	0	0	2	0
3	D	111	0	0	1	0
3	E	135	0	0	3	0
3	F	115	0	0	1	0
3	G	133	0	0	2	0
3	H	147	0	0	9	0
3	I	149	0	0	0	0
3	J	159	0	0	2	0
All	All	20960	0	19660	99	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 3.

All (99) 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:H:33[B]:ASP:CG	3:H:2018:HOH:O	2.07	0.93
1:C:144:GLU:CD	3:C:2083:HOH:O	2.21	0.78
1:G:89[B]:GLU:HG2	1:G:118:GLY:H	1.50	0.76
1:E:78:LYS:CE	1:E:144:GLU:OE2	2.34	0.75
1:H:33[A]:ASP:OD1	3:H:2018:HOH:O	2.04	0.74
1:A:28:GLU:O	1:A:84:THR:HG23	1.92	0.70
1:H:33[A]:ASP:HB2	1:H:236:GLN:NE2	2.08	0.68
1:H:33[A]:ASP:HB3	3:H:2018:HOH:O	1.94	0.65
1:A:125:GLU:OE1	1:E:122:LYS:NZ	2.28	0.65
1:G:7:LYS:HE2	3:G:2065:HOH:O	1.97	0.65
1:A:78:LYS:HE3	1:A:144:GLU:OE2	1.97	0.64
1:A:25:HIS:HE1	2:A:270:FBP:O1P	1.80	0.64
1:C:28:GLU:O	1:C:84:THR:HG23	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:33[B]:ASP:OD1	3:H:2018:HOH:O	2.09	0.63
1:E:78:LYS:HE3	1:E:144:GLU:OE2	1.99	0.62
1:J:17:LYS:NZ	3:J:2007:HOH:O	2.33	0.61
1:E:24:ASP:HB2	1:E:61:GLN:HE21	1.64	0.61
1:H:33[A]:ASP:CG	3:H:2018:HOH:O	2.38	0.60
1:H:33[A]:ASP:HB2	1:H:236:GLN:HE21	1.66	0.60
1:E:33:ASP:N	3:E:2019:HOH:O	2.34	0.59
1:F:28:GLU:O	1:F:84:THR:HG23	2.02	0.59
1:H:61:GLN:HE22	1:H:78:LYS:HZ3	1.51	0.58
1:A:125:GLU:HG3	1:E:93:VAL:HG21	1.85	0.58
1:E:78:LYS:HE2	1:E:144:GLU:OE2	2.04	0.57
1:H:125:GLU:HG3	1:I:93:VAL:HG21	1.87	0.56
1:F:24:ASP:HB2	1:F:61:GLN:HE21	1.69	0.56
1:D:24:ASP:HB2	1:D:61:GLN:HE21	1.71	0.56
1:C:24:ASP:HB2	1:C:61:GLN:HE21	1.71	0.55
1:J:24:ASP:HB2	1:J:61:GLN:HE21	1.72	0.55
1:A:232:ARG:O	1:A:236:GLN:HB2	2.07	0.54
1:A:24:ASP:HB2	1:A:61:GLN:HE21	1.73	0.54
1:B:95:ASN:HA	1:C:128:ALA:HB2	1.89	0.54
1:H:33[A]:ASP:CB	3:H:2018:HOH:O	2.54	0.54
1:D:33:ASP:HA	3:D:2016:HOH:O	2.07	0.53
1:J:48:ARG:HD3	3:J:2031:HOH:O	2.07	0.53
1:D:28:GLU:O	1:D:84:THR:HG23	2.09	0.53
1:I:28:GLU:O	1:I:84:THR:HG23	2.08	0.53
1:D:95:ASN:HA	1:E:128:ALA:HB2	1.90	0.53
1:G:128:ALA:HB2	1:H:95:ASN:HA	1.91	0.53
1:F:125:GLU:HG3	1:G:93:VAL:HG21	1.89	0.52
1:I:24:ASP:HB2	1:I:61:GLN:HE21	1.74	0.52
1:E:28:GLU:O	1:E:84:THR:HG23	2.09	0.52
1:H:24:ASP:HB2	1:H:61:GLN:HE21	1.75	0.52
1:G:28:GLU:O	1:G:84:THR:HG23	2.09	0.51
1:J:57:GLY:HA2	1:J:73:VAL:HG12	1.91	0.51
1:A:78:LYS:NZ	3:A:2040:HOH:O	2.16	0.51
1:G:89[B]:GLU:HG2	1:G:118:GLY:N	2.24	0.51
1:F:7:LYS:HE2	3:F:2056:HOH:O	2.09	0.51
1:I:61:GLN:HE22	1:I:78:LYS:HZ3	1.59	0.51
1:H:33[B]:ASP:CB	3:H:2018:HOH:O	2.51	0.50
1:F:95:ASN:HA	1:J:128:ALA:HB2	1.93	0.50
1:H:28:GLU:O	1:H:84:THR:HG23	2.11	0.50
1:A:78:LYS:CE	1:A:144:GLU:OE2	2.60	0.49
1:H:15:ARG:HD3	3:H:2040:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:ARG:HD3	1:H:72:SER:HB2	1.95	0.49
1:H:33[B]:ASP:HB2	3:H:2018:HOH:O	2.10	0.48
1:D:120:GLU:HG3	1:D:124:PHE:CE2	2.49	0.48
1:B:24:ASP:HB2	1:B:61:GLN:HE21	1.78	0.48
1:I:128:ALA:HB2	1:J:95:ASN:HA	1.95	0.48
1:J:28:GLU:O	1:J:84:THR:HG23	2.13	0.48
1:G:24:ASP:HB2	1:G:61:GLN:HE21	1.79	0.48
1:A:78:LYS:HE2	1:A:80:ASN:OD1	2.14	0.48
1:I:29:HIS:NE2	2:I:270:FBP:O4P	2.39	0.48
1:B:36:ASP:OD2	1:B:236:GLN:NE2	2.47	0.47
1:H:128:ALA:HB2	1:I:95:ASN:HA	1.96	0.47
1:C:61:GLN:HE22	1:C:78:LYS:HZ3	1.61	0.47
1:B:78:LYS:HD2	1:B:80:ASN:O	2.15	0.47
1:G:17:LYS:NZ	3:G:2015:HOH:O	2.42	0.47
1:A:95:ASN:HA	1:B:128:ALA:HB2	1.97	0.47
1:A:78:LYS:CD	1:A:144:GLU:OE2	2.63	0.46
1:F:61:GLN:HE22	1:F:78:LYS:HZ3	1.64	0.46
1:C:95:ASN:HA	1:D:128:ALA:HB2	1.98	0.46
1:B:28:GLU:O	1:B:84:THR:HG23	2.16	0.46
1:B:93:VAL:HG21	1:C:125:GLU:HG3	1.98	0.45
1:C:232:ARG:O	1:C:236:GLN:HB2	2.15	0.45
1:E:245:ARG:HD3	3:E:2132:HOH:O	2.15	0.45
1:B:146:PHE:HE2	3:B:2113:HOH:O	1.98	0.45
1:J:55:PHE:CZ	1:J:244:ALA:HB1	2.51	0.45
1:C:82:LYS:CE	3:C:2037:HOH:O	2.65	0.44
1:E:33:ASP:HA	3:E:2018:HOH:O	2.18	0.43
1:A:120:GLU:HG3	1:A:124:PHE:CE2	2.54	0.43
1:E:57:GLY:HA2	1:E:73:VAL:HG12	1.99	0.43
1:G:57:GLY:HA2	1:G:73:VAL:HG12	2.00	0.43
1:F:23:TYR:CE1	1:F:46:ILE:HG13	2.54	0.42
1:H:33[B]:ASP:CG	1:H:236:GLN:NE2	2.73	0.42
1:H:127:LEU:HD11	1:H:141:LEU:HD21	2.01	0.42
1:H:33[B]:ASP:CG	1:H:236:GLN:HE22	2.23	0.42
1:A:128:ALA:HB2	1:E:95:ASN:HA	2.01	0.42
1:A:29:HIS:NE2	2:A:270:FBP:O4P	2.42	0.42
1:D:87:ASN:HA	1:D:87:ASN:HD22	1.59	0.42
1:H:61:GLN:HE22	1:H:78:LYS:NZ	2.17	0.41
1:J:23:TYR:CE1	1:J:46:ILE:HG13	2.55	0.41
1:E:177:LYS:NZ	2:E:270:FBP:O3	2.54	0.41
1:I:120:GLU:HG3	1:I:124:PHE:CE2	2.56	0.41
1:H:109:VAL:HG13	1:H:139:LEU:HD23	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:48:ARG:HG2	1:H:51:ARG:NH2	2.37	0.41
1:H:158:PRO:HB3	1:H:186:THR:HB	2.03	0.41
1:H:29:HIS:NE2	2:H:270:FBP:O4P	2.42	0.40
1:B:68:TYR:CE1	1:C:196:LYS:HE3	2.56	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)
1:C:208:LYS:O	1:G:44:GLU:OE2[2_546]	2.13	0.07

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	251/263 (95%)	246 (98%)	5 (2%)	0	100	100
1	B	249/263 (95%)	243 (98%)	6 (2%)	0	100	100
1	C	250/263 (95%)	244 (98%)	6 (2%)	0	100	100
1	D	249/263 (95%)	244 (98%)	5 (2%)	0	100	100
1	E	252/263 (96%)	246 (98%)	6 (2%)	0	100	100
1	F	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
1	G	252/263 (96%)	247 (98%)	5 (2%)	0	100	100
1	H	252/263 (96%)	246 (98%)	6 (2%)	0	100	100
1	I	250/263 (95%)	245 (98%)	5 (2%)	0	100	100
1	J	252/263 (96%)	247 (98%)	5 (2%)	0	100	100
All	All	2507/2630 (95%)	2453 (98%)	54 (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	200/206 (97%)	190 (95%)	10 (5%)	30	11
1	B	198/206 (96%)	191 (96%)	7 (4%)	43	23
1	C	199/206 (97%)	191 (96%)	8 (4%)	38	18
1	D	198/206 (96%)	187 (94%)	11 (6%)	26	9
1	E	199/206 (97%)	190 (96%)	9 (4%)	34	14
1	F	199/206 (97%)	189 (95%)	10 (5%)	30	11
1	G	201/206 (98%)	194 (96%)	7 (4%)	43	23
1	H	201/206 (98%)	191 (95%)	10 (5%)	30	11
1	I	199/206 (97%)	193 (97%)	6 (3%)	48	29
1	J	201/206 (98%)	196 (98%)	5 (2%)	55	37
All	All	1995/2060 (97%)	1912 (96%)	83 (4%)	37	16

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	51	ARG
1	A	77	LEU
1	A	120	GLU
1	A	139	LEU
1	A	163	TYR
1	A	201	MET
1	A	218[A]	GLU
1	A	218[B]	GLU
1	A	245	ARG
1	B	77	LEU
1	B	78	LYS
1	B	139	LEU
1	B	163	TYR
1	B	183	ASP
1	B	201	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	222	GLU
1	C	14	ARG
1	C	35	MET
1	C	51	ARG
1	C	77	LEU
1	C	139	LEU
1	C	163	TYR
1	C	201	MET
1	C	238	ARG
1	D	14	ARG
1	D	77	LEU
1	D	87	ASN
1	D	120	GLU
1	D	139	LEU
1	D	163	TYR
1	D	201	MET
1	D	208	LYS
1	D	215	LYS
1	D	238	ARG
1	D	245	ARG
1	E	14	ARG
1	E	35[A]	MET
1	E	35[B]	MET
1	E	51	ARG
1	E	77	LEU
1	E	163	TYR
1	E	183	ASP
1	E	201	MET
1	E	208	LYS
1	F	35[A]	MET
1	F	35[B]	MET
1	F	77	LEU
1	F	120	GLU
1	F	139	LEU
1	F	163	TYR
1	F	179	LYS
1	F	183	ASP
1	F	201	MET
1	F	238	ARG
1	G	48	ARG
1	G	77	LEU
1	G	78	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	139	LEU
1	G	163	TYR
1	G	201	MET
1	G	208	LYS
1	H	14	ARG
1	H	15	ARG
1	H	77	LEU
1	H	139	LEU
1	H	163	TYR
1	H	185	LYS
1	H	201	MET
1	H	208	LYS
1	H	215	LYS
1	H	238	ARG
1	I	77	LEU
1	I	120	GLU
1	I	139	LEU
1	I	163	TYR
1	I	201	MET
1	I	249	GLU
1	J	14	ARG
1	J	77	LEU
1	J	139	LEU
1	J	163	TYR
1	J	201	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	61	GLN
1	B	61	GLN
1	C	61	GLN
1	D	61	GLN
1	D	87	ASN
1	E	61	GLN
1	F	61	GLN
1	G	61	GLN
1	H	61	GLN
1	H	236	GLN
1	I	61	GLN
1	J	61	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	FBP	A	270	-	18,20,20	0.86	1 (5%)	21,32,32	1.09	1 (4%)
2	FBP	B	270	-	18,20,20	1.00	1 (5%)	21,32,32	0.64	0
2	FBP	C	270	-	18,20,20	0.99	1 (5%)	21,32,32	0.96	2 (9%)
2	FBP	D	270	-	18,20,20	0.88	1 (5%)	21,32,32	0.69	0
2	FBP	E	270	-	18,20,20	0.69	1 (5%)	21,32,32	0.96	1 (4%)
2	FBP	F	270	-	18,20,20	0.86	1 (5%)	21,32,32	0.87	0
2	FBP	G	270	-	18,20,20	0.73	0	21,32,32	0.66	0
2	FBP	H	270	-	18,20,20	0.95	1 (5%)	21,32,32	1.00	1 (4%)
2	FBP	I	270	-	18,20,20	0.81	1 (5%)	21,32,32	1.31	5 (23%)
2	FBP	J	270	-	18,20,20	0.96	1 (5%)	21,32,32	0.67	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	FBP	A	270	-	-	0/13/32/32	0/1/1/1
2	FBP	B	270	-	-	0/13/32/32	0/1/1/1
2	FBP	C	270	-	-	0/13/32/32	0/1/1/1
2	FBP	D	270	-	-	0/13/32/32	0/1/1/1
2	FBP	E	270	-	-	0/13/32/32	0/1/1/1
2	FBP	F	270	-	-	0/13/32/32	0/1/1/1
2	FBP	G	270	-	-	0/13/32/32	0/1/1/1
2	FBP	H	270	-	-	0/13/32/32	0/1/1/1
2	FBP	I	270	-	-	0/13/32/32	0/1/1/1
2	FBP	J	270	-	-	0/13/32/32	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	270	FBP	O3-C3	-2.00	1.38	1.42
2	A	270	FBP	O2-C2	2.07	1.44	1.41
2	I	270	FBP	O2-C2	2.11	1.44	1.41
2	F	270	FBP	O2-C2	2.36	1.44	1.41
2	E	270	FBP	O2-C2	2.41	1.45	1.41
2	D	270	FBP	O2-C2	2.76	1.45	1.41
2	C	270	FBP	O2-C2	3.08	1.46	1.41
2	J	270	FBP	O2-C2	3.10	1.46	1.41
2	B	270	FBP	O2-C2	3.14	1.46	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	270	FBP	O5P-P2-O4P	-2.22	103.44	110.58
2	C	270	FBP	O5P-P2-O4P	-2.17	103.59	110.58
2	E	270	FBP	O6P-P2-O4P	-2.05	103.97	110.58
2	I	270	FBP	O6P-P2-O6	-2.02	100.75	106.56
2	I	270	FBP	O3P-P1-O1	2.09	112.57	106.56
2	I	270	FBP	O6-P2-O4P	2.18	112.68	107.14
2	H	270	FBP	O5P-P2-O6	2.26	113.07	106.56
2	C	270	FBP	O5P-P2-O6	2.53	113.86	106.56
2	A	270	FBP	O5P-P2-O6	2.54	113.88	106.56
2	I	270	FBP	O5P-P2-O6	2.73	114.42	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	270	FBP	2	0
2	E	270	FBP	1	0
2	H	270	FBP	1	0
2	I	270	FBP	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

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, 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	A	250/263 (95%)	0.21	9 (3%) 46 44	11, 14, 22, 28	0
1	B	250/263 (95%)	0.11	7 (2%) 56 54	11, 14, 22, 26	0
1	C	250/263 (95%)	0.36	22 (8%) 12 12	11, 15, 22, 28	0
1	D	250/263 (95%)	0.06	10 (4%) 42 39	11, 14, 22, 25	0
1	E	252/263 (95%)	0.16	9 (3%) 46 44	11, 14, 22, 28	0
1	F	250/263 (95%)	0.21	14 (5%) 28 26	11, 15, 21, 29	0
1	G	250/263 (95%)	-0.03	4 (1%) 74 74	10, 14, 22, 30	0
1	H	250/263 (95%)	0.15	10 (4%) 42 39	10, 15, 21, 27	0
1	I	250/263 (95%)	0.15	8 (3%) 51 48	11, 14, 22, 27	0
1	J	250/263 (95%)	-0.04	3 (1%) 81 81	11, 14, 22, 28	0
All	All	2502/2630 (95%)	0.13	96 (3%) 44 41	10, 14, 22, 30	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	254	GLY	4.8
1	D	208	LYS	4.4
1	C	238	ARG	4.2
1	C	214	LEU	3.6
1	F	238	ARG	3.6
1	E	238	ARG	3.5
1	F	249	GLU	3.5
1	A	238	ARG	3.3
1	C	209	THR	3.3
1	C	250	LEU	3.2
1	H	238	ARG	3.2
1	J	208	LYS	3.2
1	F	215	LYS	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	211	GLU	3.2
1	H	243	PHE	3.2
1	C	243	PHE	3.1
1	B	143	VAL	3.1
1	F	182	GLY	3.1
1	C	252	TYR	3.0
1	D	211	GLU	3.0
1	C	218	GLU	3.0
1	C	249	GLU	3.0
1	C	213	PHE	3.0
1	H	208	LYS	2.9
1	H	214	LEU	2.9
1	C	208	LYS	2.8
1	D	247	LEU	2.8
1	C	211	GLU	2.8
1	E	113	ILE	2.8
1	A	142	VAL	2.8
1	E	208	LYS	2.8
1	C	215	LYS	2.7
1	A	79	LEU	2.7
1	I	249	GLU	2.7
1	D	212	ASP	2.7
1	G	113	ILE	2.7
1	I	143	VAL	2.7
1	F	208	LYS	2.7
1	C	251	VAL	2.7
1	F	214	LEU	2.7
1	H	36	ASP	2.6
1	F	212	ASP	2.6
1	H	143	VAL	2.6
1	I	111	TYR	2.6
1	C	35	MET	2.5
1	B	171	LEU	2.5
1	C	240	ALA	2.5
1	C	222	GLU	2.5
1	H	182	GLY	2.5
1	F	213	PHE	2.5
1	I	142	VAL	2.5
1	J	211	GLU	2.4
1	D	209	THR	2.4
1	I	171	LEU	2.4
1	D	14	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	36	ASP	2.4
1	F	250	LEU	2.4
1	A	211	GLU	2.4
1	H	211	GLU	2.4
1	B	127	LEU	2.3
1	G	208	LYS	2.3
1	D	215	LYS	2.3
1	F	38	PRO	2.3
1	I	113	ILE	2.3
1	B	215	LYS	2.3
1	C	49	LEU	2.2
1	J	238	ARG	2.2
1	D	185	LYS	2.2
1	C	246	ALA	2.2
1	E	143	VAL	2.2
1	H	242	LYS	2.2
1	B	113	ILE	2.2
1	H	27	ILE	2.2
1	A	77	LEU	2.2
1	B	142	VAL	2.2
1	E	142	VAL	2.2
1	D	214	LEU	2.2
1	E	209	THR	2.2
1	A	35[A]	MET	2.2
1	E	211	GLU	2.1
1	F	184	PRO	2.1
1	G	238	ARG	2.1
1	B	169	LEU	2.1
1	A	249	GLU	2.1
1	F	209	THR	2.1
1	C	212	ASP	2.1
1	I	79	LEU	2.1
1	D	218	GLU	2.1
1	A	94	ALA	2.1
1	C	247	LEU	2.1
1	A	93	VAL	2.1
1	C	171	LEU	2.0
1	G	171	LEU	2.0
1	I	141	LEU	2.0
1	C	220	VAL	2.0
1	F	251	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FBP	I	270	20/20	0.95	0.10	0.22	12,25,36,38	0
2	FBP	D	270	20/20	0.95	0.09	-0.15	12,25,36,37	0
2	FBP	C	270	20/20	0.93	0.11	-0.19	13,24,34,36	0
2	FBP	G	270	20/20	0.95	0.09	-0.27	11,23,33,33	0
2	FBP	B	270	20/20	0.96	0.10	-0.28	14,23,36,36	0
2	FBP	J	270	20/20	0.95	0.09	-0.32	16,24,34,35	0
2	FBP	A	270	20/20	0.95	0.09	-0.48	12,26,35,36	0
2	FBP	E	270	20/20	0.95	0.08	-0.53	14,26,34,35	0
2	FBP	H	270	20/20	0.97	0.08	-0.59	13,24,37,39	0
2	FBP	F	270	20/20	0.96	0.08	-0.73	14,23,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.