Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2024 – 08:04 PM EST

PDB ID	:	6PFK
Title	:	PHOSPHOFRUCTOKINASE, INHIBITED T-STATE
Authors	:	Evans, P.R.; Schirmer, T.; Auer, M.
Deposited on	:	1996-01-04
Resolution	:	2.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

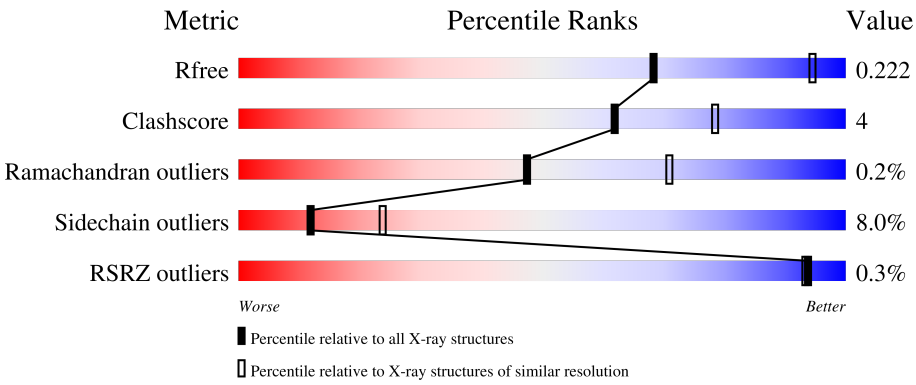
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	319	% 73% 22% • •
1	B	319	73% 22% 5% •
1	C	319	77% 19% • •
1	D	319	75% 21% • •

2 Entry composition (i)

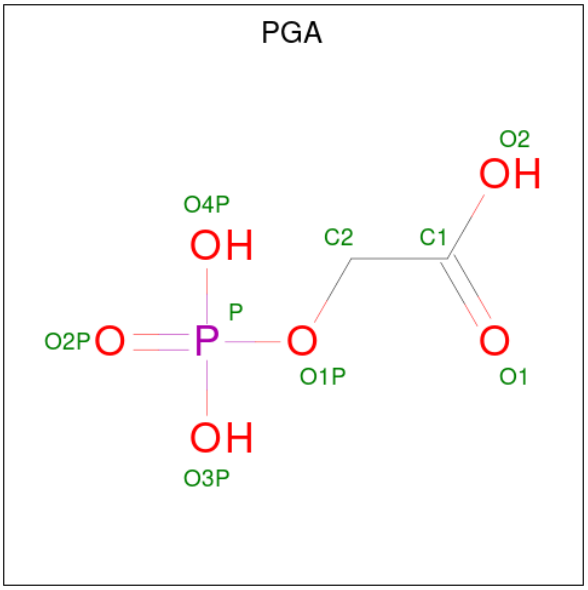
There are 3 unique types of molecules in this entry. The entry contains 9681 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHOFRUCTOKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2341	1466	420	447	8	0	1	0
1	B	319	2349	1470	422	449	8	0	1	0
1	C	319	2355	1473	420	454	8	0	1	0
1	D	319	2374	1486	425	455	8	0	1	0

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula: $C_2H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	9	2	6	1	0	0
2	B	1	9	2	6	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	C	1	9	2	6	1	0	0
			Total	C	O	P		
2	D	1	9	2	6	1	0	0

- Molecule 3 is water.

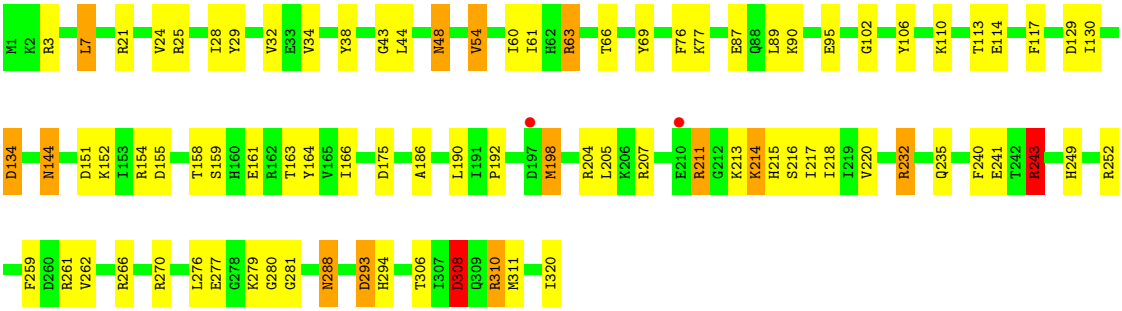
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	53	53	53	0	0
			Total	O		
3	B	59	59	59	0	0
			Total	O		
3	C	50	50	50	0	0
			Total	O		
3	D	64	64	64	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

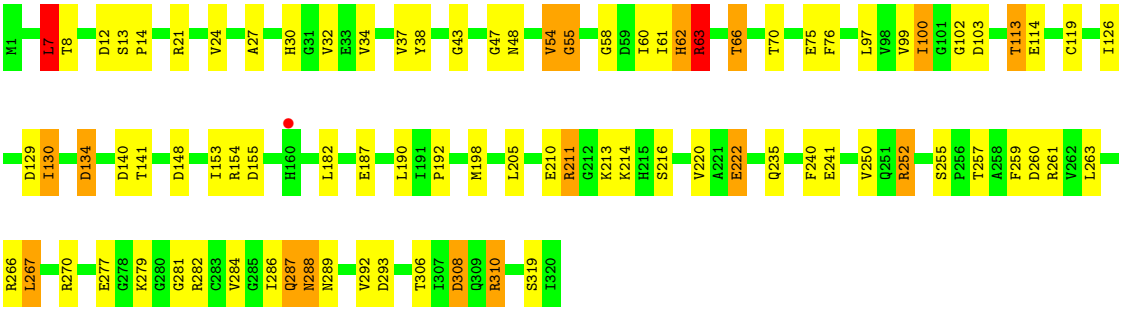
• Molecule 1: PHOSPHOFRUCTOKINASE

Chain A:



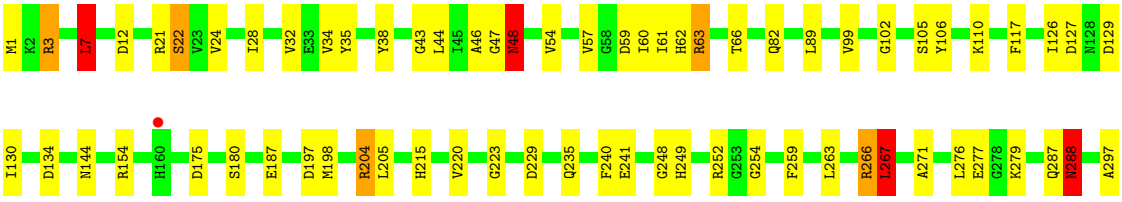
• Molecule 1: PHOSPHOFRUCTOKINASE

Chain B:



• Molecule 1: PHOSPHOFRUCTOKINASE

Chain C:



• Molecule 1: PHOSPHOFRUCTOKINASE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	132.00Å 115.20Å 96.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 19.82 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.0 (15.00-2.60) 97.0 (19.82-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.59Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.255 0.160 , 0.222	Depositor DCC
R_{free} test set	2242 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9681	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 (i)

5.1 Standard geometry (i)

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

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	0.64	0/2383	1.92	65/3226 (2.0%)
1	B	0.65	0/2391	1.89	61/3235 (1.9%)
1	C	0.62	0/2397	1.89	49/3242 (1.5%)
1	D	0.68	0/2416	1.96	55/3263 (1.7%)
All	All	0.65	0/9587	1.92	230/12966 (1.8%)

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	0	8
1	B	0	8
1	C	0	1
1	D	0	9
All	All	0	26

There are no bond length outliers.

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	232	ARG	CD-NE-CZ	27.44	162.01	123.60
1	B	310	ARG	NE-CZ-NH1	17.67	129.13	120.30
1	D	232	ARG	NE-CZ-NH1	17.36	128.98	120.30
1	D	252	ARG	NE-CZ-NH2	-17.31	111.64	120.30
1	C	252	ARG	NE-CZ-NH2	-16.45	112.07	120.30
1	A	310	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	B	252	ARG	NE-CZ-NH2	-15.11	112.75	120.30
1	B	211	ARG	CD-NE-CZ	14.78	144.29	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	211	ARG	CD-NE-CZ	14.55	143.97	123.60
1	D	232	ARG	NE-CZ-NH2	-14.54	113.03	120.30
1	C	252	ARG	NE-CZ-NH1	14.06	127.33	120.30
1	C	310	ARG	NE-CZ-NH1	13.78	127.19	120.30
1	A	21	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	C	310	ARG	NE-CZ-NH2	-13.45	113.57	120.30
1	A	266	ARG	NE-CZ-NH2	-13.23	113.68	120.30
1	A	154	ARG	NE-CZ-NH2	-12.94	113.83	120.30
1	B	310	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	B	252	ARG	NE-CZ-NH1	10.59	125.60	120.30
1	A	308	ASP	CB-CG-OD1	10.57	127.81	118.30
1	D	7	LEU	CA-CB-CG	10.56	139.58	115.30
1	C	266	ARG	NE-CZ-NH2	-10.47	115.06	120.30
1	D	287	GLN	N-CA-CB	9.58	127.85	110.60
1	D	310	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	B	140	ASP	CB-CG-OD1	9.30	126.67	118.30
1	A	232	ARG	NE-CZ-NH2	-9.05	115.78	120.30
1	B	21	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	A	232	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	243	ARG	CD-NE-CZ	8.82	135.95	123.60
1	C	12	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	C	310	ARG	CD-NE-CZ	8.68	135.75	123.60
1	A	243	ARG	CG-CD-NE	8.61	129.89	111.80
1	D	252	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	D	236	GLU	OE1-CD-OE2	8.31	133.28	123.30
1	C	21	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	C	154	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	7	LEU	CA-CB-CG	8.09	133.90	115.30
1	B	310	ARG	CD-NE-CZ	8.03	134.84	123.60
1	C	300	LEU	O-C-N	-7.97	109.94	122.70
1	D	266	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	61	ILE	C-N-CA	7.81	141.23	121.70
1	B	103	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	B	261	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	252	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	B	270	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	154	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	C	134	ASP	CB-CG-OD2	7.53	125.08	118.30
1	C	7	LEU	CA-CB-CG	7.51	132.58	115.30
1	D	12	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	D	106	TYR	CB-CG-CD1	7.39	125.44	121.00
1	B	129	ASP	CA-C-O	7.33	135.49	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	21	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	153	ILE	O-C-N	-7.21	111.16	122.70
1	B	255	SER	N-CA-CB	-7.21	99.68	110.50
1	D	204	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	D	61	ILE	C-N-CA	7.07	139.37	121.70
1	C	300	LEU	C-N-CA	7.04	139.31	121.70
1	D	12	ASP	CB-CG-OD1	7.00	124.60	118.30
1	C	288	ASN	O-C-N	-6.98	111.53	122.70
1	A	63	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	270	ARG	CD-NE-CZ	6.90	133.26	123.60
1	A	261	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	192	PRO	C-N-CA	6.87	138.88	121.70
1	D	127	ASP	CB-CA-C	-6.84	96.73	110.40
1	B	54	VAL	CB-CA-C	-6.83	98.42	111.40
1	A	7	LEU	CA-CB-CG	6.78	130.90	115.30
1	D	106	TYR	CB-CG-CD2	-6.78	116.93	121.00
1	D	129	ASP	O-C-N	-6.75	111.89	122.70
1	A	163	THR	CA-C-O	6.72	134.21	120.10
1	B	61	ILE	C-N-CA	6.68	138.40	121.70
1	B	266	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	C	267	LEU	O-C-N	-6.63	111.93	123.20
1	C	28	ILE	O-C-N	-6.61	112.12	122.70
1	A	134	ASP	O-C-N	-6.55	112.22	122.70
1	B	114	GLU	O-C-N	-6.49	112.31	122.70
1	C	129	ASP	CA-C-O	6.44	133.63	120.10
1	A	164	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	D	7	LEU	CB-CG-CD2	6.42	121.92	111.00
1	C	249	HIS	C-N-CA	6.38	137.66	121.70
1	D	129	ASP	CA-C-O	6.36	133.46	120.10
1	C	61	ILE	C-N-CA	6.31	137.47	121.70
1	B	63	ARG	CB-CG-CD	6.31	128.00	111.60
1	B	114	GLU	C-N-CA	6.30	137.45	121.70
1	A	277	GLU	O-C-N	-6.28	112.52	123.20
1	A	61	ILE	O-C-N	-6.26	112.68	122.70
1	A	25	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	204	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	3	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	249	HIS	O-C-N	-6.21	112.77	122.70
1	A	249	HIS	C-N-CA	6.17	137.11	121.70
1	C	198	MET	C-N-CA	6.17	137.11	121.70
1	C	127	ASP	CB-CA-C	-6.12	98.15	110.40
1	B	222	GLU	OE1-CD-OE2	6.12	130.64	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	211	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	129	ASP	O-C-N	-6.08	112.97	122.70
1	B	155	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	54	VAL	CB-CA-C	-6.05	99.90	111.40
1	B	211	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	46	ALA	CA-C-N	6.03	128.27	116.20
1	B	277	GLU	O-C-N	-6.01	112.98	123.20
1	A	310	ARG	CD-NE-CZ	6.01	132.02	123.60
1	C	180	SER	CB-CA-C	-5.98	98.73	110.10
1	C	271	ALA	O-C-N	-5.96	113.16	122.70
1	C	144	ASN	O-C-N	-5.95	113.18	122.70
1	D	54	VAL	CB-CA-C	-5.94	100.11	111.40
1	B	134	ASP	O-C-N	-5.92	113.23	122.70
1	C	35	TYR	CG-CD1-CE1	5.90	126.02	121.30
1	A	308	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	103	ASP	OD1-CG-OD2	5.89	134.50	123.30
1	D	240	PHE	CB-CG-CD1	5.87	124.91	120.80
1	A	240	PHE	CB-CG-CD1	5.86	124.90	120.80
1	C	277	GLU	CA-CB-CG	5.85	126.28	113.40
1	D	197	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	D	55	GLY	O-C-N	-5.83	113.37	122.70
1	B	277	GLU	C-N-CA	5.82	134.52	122.30
1	C	229	ASP	CB-CG-OD1	5.80	123.52	118.30
1	D	114	GLU	C-N-CA	5.79	136.17	121.70
1	D	35	TYR	CG-CD1-CE1	5.79	125.93	121.30
1	C	254	GLY	CA-C-O	5.78	131.00	120.60
1	B	260	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	154	ARG	CA-C-N	5.76	129.86	117.20
1	D	289	ASN	C-N-CA	5.74	136.06	121.70
1	B	192	PRO	C-N-CA	5.73	136.02	121.70
1	D	22	SER	CA-C-N	5.72	129.79	117.20
1	B	153	ILE	CA-C-N	5.72	129.79	117.20
1	D	277	GLU	O-C-N	-5.72	113.47	123.20
1	D	120	VAL	C-N-CA	5.72	134.31	122.30
1	C	63	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	D	222	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	D	169	MET	CA-CB-CG	-5.70	103.61	113.30
1	D	249	HIS	C-N-CA	5.69	135.92	121.70
1	D	310	ARG	CD-NE-CZ	5.69	131.56	123.60
1	D	214	LYS	O-C-N	-5.68	113.61	122.70
1	A	129	ASP	CA-C-O	5.66	131.99	120.10
1	A	288	ASN	O-C-N	-5.66	113.64	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	7	LEU	CB-CG-CD2	5.66	120.62	111.00
1	A	106	TYR	CB-CG-CD1	5.66	124.39	121.00
1	D	59	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	48	ASN	C-N-CA	5.65	135.82	121.70
1	B	12	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	148	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	186	ALA	N-CA-CB	5.62	117.97	110.10
1	A	198	MET	C-N-CA	5.61	135.73	121.70
1	A	294	HIS	CB-CA-C	-5.60	99.19	110.40
1	C	249	HIS	O-C-N	-5.59	113.75	122.70
1	D	30	HIS	O-C-N	-5.58	113.71	123.20
1	A	293	ASP	O-C-N	-5.57	113.78	122.70
1	C	106	TYR	CB-CG-CD1	5.57	124.34	121.00
1	A	279	LYS	O-C-N	-5.56	113.74	123.20
1	B	240	PHE	CB-CG-CD1	5.55	124.68	120.80
1	D	59	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	250	VAL	O-C-N	-5.54	113.84	122.70
1	C	198	MET	O-C-N	-5.53	113.85	122.70
1	B	103	ASP	CA-CB-CG	-5.52	101.25	113.40
1	D	145	THR	CA-CB-OG1	-5.52	97.41	109.00
1	B	55	GLY	O-C-N	-5.51	113.88	122.70
1	B	61	ILE	O-C-N	-5.51	113.89	122.70
1	B	277	GLU	N-CA-CB	-5.50	100.69	110.60
1	B	154	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	C	48	ASN	O-C-N	-5.50	113.91	122.70
1	A	95	GLU	OE1-CD-OE2	-5.49	116.71	123.30
1	B	289	ASN	O-C-N	-5.49	113.91	122.70
1	A	29	TYR	C-N-CA	5.48	135.40	121.70
1	D	180	SER	CB-CA-C	-5.48	99.70	110.10
1	A	214	LYS	O-C-N	-5.47	113.95	122.70
1	B	30	HIS	O-C-N	-5.46	113.91	123.20
1	B	55	GLY	CA-C-N	5.46	129.21	117.20
1	C	240	PHE	CB-CG-CD1	5.46	124.62	120.80
1	D	288	ASN	O-C-N	-5.45	113.98	122.70
1	A	218	ILE	CA-CB-CG1	5.44	121.33	111.00
1	C	59	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	48	ASN	N-CA-CB	-5.43	100.83	110.60
1	D	113	THR	O-C-N	-5.40	114.06	122.70
1	C	220	VAL	CG1-CB-CG2	-5.40	102.26	110.90
1	D	252	ARG	CG-CD-NE	-5.39	100.47	111.80
1	B	130	ILE	N-CA-C	-5.39	96.46	111.00
1	D	222	GLU	CA-C-N	5.38	126.96	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	GLN	N-CA-CB	5.37	120.27	110.60
1	D	114	GLU	O-C-N	-5.37	114.10	122.70
1	A	218	ILE	CB-CG1-CD1	5.37	128.93	113.90
1	B	308	ASP	O-C-N	-5.36	114.13	122.70
1	B	270	ARG	O-C-N	-5.35	114.14	122.70
1	A	211	ARG	CA-CB-CG	5.35	125.16	113.40
1	B	75	GLU	O-C-N	-5.35	114.15	122.70
1	C	197	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	21	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	204	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	266	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	3	ARG	CB-CA-C	-5.33	99.73	110.40
1	A	207	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	259[A]	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	D	259[B]	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	A	215	HIS	N-CA-CB	5.31	120.16	110.60
1	A	114	GLU	CA-C-N	5.30	128.87	117.20
1	D	192	PRO	C-N-CA	5.29	134.94	121.70
1	A	151	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	144	ASN	CB-CA-C	5.28	120.97	110.40
1	B	100	ILE	CB-CG1-CD1	5.28	128.67	113.90
1	B	216	SER	N-CA-CB	5.27	118.41	110.50
1	A	106	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	B	155	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	D	222	GLU	O-C-N	-5.25	114.27	123.20
1	C	287	GLN	N-CA-CB	5.25	120.04	110.60
1	B	103	ASP	CB-CA-C	-5.22	99.96	110.40
1	B	288	ASN	C-N-CA	5.21	134.73	121.70
1	C	3	ARG	CG-CD-NE	5.21	122.74	111.80
1	A	155	ASP	CA-C-N	5.21	128.66	117.20
1	C	129	ASP	O-C-N	-5.20	114.38	122.70
1	A	77	LYS	C-N-CA	5.17	134.63	121.70
1	D	78	THR	CA-C-O	5.17	130.95	120.10
1	D	130	ILE	N-CA-C	-5.16	97.08	111.00
1	C	12	ASP	CB-CG-OD1	5.15	122.94	118.30
1	D	32	VAL	CA-CB-CG1	5.15	118.62	110.90
1	C	47	GLY	C-N-CA	5.14	134.55	121.70
1	D	310	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	29	TYR	O-C-N	-5.12	114.50	122.70
1	A	163	THR	O-C-N	-5.10	114.53	122.70
1	C	223	GLY	C-N-CA	5.10	134.45	121.70
1	C	126	ILE	C-N-CA	5.10	134.44	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	28	ILE	O-C-N	-5.09	114.56	122.70
1	B	58	GLY	O-C-N	-5.09	114.56	122.70
1	A	310	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	257	THR	CA-CB-CG2	5.08	119.51	112.40
1	C	248	GLY	O-C-N	-5.07	114.59	122.70
1	B	277	GLU	CB-CA-C	5.07	120.53	110.40
1	B	282	ARG	CA-CB-CG	5.06	124.53	113.40
1	B	47	GLY	O-C-N	-5.05	114.62	122.70
1	D	69	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	C	7	LEU	CB-CG-CD2	5.02	119.54	111.00
1	A	134	ASP	C-N-CA	5.01	134.22	121.70
1	A	216	SER	N-CA-CB	5.01	118.01	110.50

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ASP	Mainchain
1	A	144	ASN	Mainchain
1	A	214	LYS	Mainchain
1	A	280	GLY	Mainchain
1	A	288	ASN	Mainchain
1	A	293	ASP	Mainchain
1	A	308	ASP	Mainchain
1	A	90	LYS	Mainchain
1	B	113	THR	Mainchain
1	B	134	ASP	Mainchain
1	B	214	LYS	Mainchain
1	B	288	ASN	Mainchain
1	B	293	ASP	Mainchain
1	B	308	ASP	Mainchain
1	B	55	GLY	Mainchain
1	B	66	THR	Mainchain
1	C	288	ASN	Mainchain
1	D	113	THR	Mainchain
1	D	134	ASP	Mainchain
1	D	152	LYS	Mainchain
1	D	214	LYS	Mainchain
1	D	238	THR	Mainchain
1	D	288	ASN	Mainchain
1	D	293	ASP	Mainchain
1	D	55	GLY	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	74	PRO	Mainchain

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	2341	0	2283	24	0
1	B	2349	0	2302	29	0
1	C	2355	0	2305	23	0
1	D	2374	0	2349	26	0
2	A	9	0	2	0	0
2	B	9	0	2	0	0
2	C	9	0	2	0	0
2	D	9	0	2	0	0
3	A	53	0	0	0	0
3	B	59	0	0	0	0
3	C	50	0	0	1	0
3	D	64	0	0	1	0
All	All	9681	0	9247	83	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 4.

All (83) 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:259[B]:PHE:CD2	1:B:259[B]:PHE:CD2	2.62	0.88
1:A:259[B]:PHE:HD2	1:B:259[B]:PHE:CE2	1.93	0.85
1:A:259[B]:PHE:CD2	1:B:259[B]:PHE:HD2	1.95	0.84
1:C:259[B]:PHE:CE2	1:D:259[B]:PHE:HD2	1.97	0.83
1:A:259[B]:PHE:CE2	1:B:259[B]:PHE:HD2	1.97	0.82
1:A:259[B]:PHE:HD2	1:B:259[B]:PHE:CD2	1.97	0.81
1:B:102:GLY:HA2	1:B:130:ILE:HD11	1.63	0.80
1:C:259[B]:PHE:CD2	1:D:259[B]:PHE:CD2	2.70	0.80
1:C:259[B]:PHE:HD2	1:D:259[B]:PHE:CE2	2.01	0.79
1:C:24:VAL:HA	1:C:34:VAL:HG21	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLY:HA2	1:A:130:ILE:HD11	1.71	0.71
1:C:259[B]:PHE:CE2	1:D:259[B]:PHE:CD2	2.81	0.69
1:D:102:GLY:HA2	1:D:130:ILE:HD11	1.75	0.69
1:C:235:GLN:HE21	1:C:241:GLU:HA	1.56	0.68
1:B:190:LEU:HD12	1:B:220:VAL:HG22	1.76	0.67
1:C:102:GLY:HA2	1:C:130:ILE:HD11	1.77	0.66
1:C:259[B]:PHE:HD2	1:D:259[B]:PHE:CD2	2.14	0.65
1:B:287:GLN:HG3	1:B:292:VAL:HG21	1.78	0.64
1:D:24:VAL:HA	1:D:34:VAL:HG21	1.81	0.62
1:A:24:VAL:HA	1:A:34:VAL:HG21	1.82	0.62
1:C:259[B]:PHE:HE2	1:D:259[B]:PHE:HD2	1.45	0.61
1:C:187:GLU:HG2	1:C:204:ARG:HD2	1.83	0.61
1:C:266:ARG:HD2	1:D:311:MET:HE3	1.82	0.60
1:B:7:LEU:HD22	1:B:99:VAL:HG22	1.86	0.58
1:C:259[B]:PHE:CD2	1:D:259[B]:PHE:CE2	2.86	0.56
1:B:24:VAL:HA	1:B:34:VAL:HG21	1.87	0.55
1:A:259[B]:PHE:CE2	1:B:259[B]:PHE:CD2	2.85	0.55
1:A:262:VAL:HG13	1:B:182:LEU:HD23	1.89	0.55
1:D:187:GLU:HG2	1:D:204:ARG:HD2	1.89	0.54
1:A:259[B]:PHE:CD2	1:B:259[B]:PHE:CE2	2.83	0.54
1:B:113:THR:HG21	1:B:281:GLY:HA2	1.91	0.53
1:A:259[B]:PHE:HD2	1:B:259[B]:PHE:HE2	1.53	0.53
1:A:190:LEU:HD12	1:A:220:VAL:HG22	1.91	0.51
1:B:60:ILE:HA	1:B:63:ARG:HG3	1.92	0.51
1:C:7:LEU:HD22	1:C:99:VAL:HG22	1.92	0.51
1:B:14:PRO:HG2	1:B:141:THR:HB	1.92	0.51
1:D:79:GLU:HG3	1:D:83:LYS:HE3	1.92	0.51
1:C:22:SER:HA	1:D:318:LEU:HD22	1.92	0.51
1:C:263:LEU:HG	1:C:267:LEU:HD22	1.93	0.51
1:C:235:GLN:NE2	1:C:241:GLU:HA	2.26	0.49
1:A:32:VAL:HG21	1:A:276:LEU:HD21	1.94	0.49
1:B:8:THR:HG22	1:B:100:ILE:HB	1.94	0.48
1:B:7:LEU:HB2	1:B:37:VAL:HB	1.94	0.48
1:A:44:LEU:HD11	1:A:89:LEU:HG	1.95	0.48
1:A:235:GLN:HE21	1:A:241:GLU:HA	1.79	0.48
1:C:44:LEU:HD11	1:C:89:LEU:HG	1.96	0.48
1:A:60:ILE:HA	1:A:63:ARG:HG3	1.95	0.48
1:C:32:VAL:HG21	1:C:276:LEU:HD21	1.97	0.46
1:A:113:THR:HG21	1:A:281:GLY:HA2	1.96	0.46
1:D:49:ILE:HD12	1:D:92:HIS:ND1	2.30	0.46
1:D:113:THR:HG22	1:D:119:CYS:H	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ARG:HA	1:A:243:ARG:HD3	1.89	0.46
1:D:86:ILE:HG23	1:D:117:PHE:CE2	2.51	0.46
1:D:204:ARG:HD3	3:D:371:HOH:O	2.15	0.45
1:D:13:SER:HB2	1:D:14:PRO:HD2	1.98	0.45
1:D:109:ALA:O	1:D:113:THR:HG23	2.16	0.45
1:D:32:VAL:HG21	1:D:276:LEU:HD21	1.97	0.45
1:A:235:GLN:NE2	1:A:241:GLU:HA	2.32	0.45
1:C:110:LYS:HD2	1:C:297:ALA:HB2	1.99	0.45
1:D:79:GLU:O	1:D:83:LYS:HG2	2.16	0.45
1:B:38:TYR:O	1:B:43:GLY:HA3	2.17	0.44
1:B:267:LEU:HG	1:B:284:VAL:HG23	1.99	0.44
1:C:204:ARG:HD3	3:C:361:HOH:O	2.16	0.44
1:D:62:HIS:CD2	1:D:62:HIS:H	2.35	0.44
1:B:97:LEU:HB3	1:B:119:CYS:SG	2.58	0.44
1:A:158:THR:HG22	1:A:161:GLU:H	1.83	0.43
1:A:38:TYR:O	1:A:43:GLY:HA3	2.18	0.43
1:D:7:LEU:HB2	1:D:37:VAL:HB	2.01	0.43
1:C:38:TYR:O	1:C:43:GLY:HA3	2.19	0.43
1:C:62:HIS:CD2	1:C:62:HIS:H	2.36	0.43
1:B:27:ALA:HB1	1:B:32:VAL:HB	2.00	0.43
1:B:62:HIS:CD2	1:B:62:HIS:H	2.36	0.43
1:A:308:ASP:HB3	1:A:311:MET:HB2	2.01	0.42
1:A:152:LYS:HD2	1:D:250:VAL:HG13	2.02	0.42
1:B:235:GLN:NE2	1:B:241:GLU:HA	2.34	0.42
1:B:13:SER:HB2	1:B:126:ILE:HG23	2.01	0.42
1:D:263:LEU:HG	1:D:267:LEU:HD22	2.02	0.41
1:D:38:TYR:O	1:D:43:GLY:HA3	2.20	0.41
1:A:166:ILE:HD13	1:A:217:ILE:HG23	2.02	0.41
1:B:263:LEU:HG	1:B:267:LEU:HD22	2.03	0.41
1:C:57:VAL:O	1:C:60:ILE:HG12	2.20	0.41
1:B:113:THR:HG21	1:B:281:GLY:CA	2.51	0.41
1:B:187:GLU:HB2	1:B:213:LYS:NZ	2.36	0.41

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	318/319 (100%)	307 (96%)	10 (3%)	1 (0%)	41	64
1	B	318/319 (100%)	308 (97%)	10 (3%)	0	100	100
1	C	318/319 (100%)	300 (94%)	17 (5%)	1 (0%)	41	64
1	D	318/319 (100%)	306 (96%)	11 (4%)	1 (0%)	41	64
All	All	1272/1276 (100%)	1221 (96%)	48 (4%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	48	ASN
1	A	69	TYR
1	D	170	GLY

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	231/247 (94%)	212 (92%)	19 (8%)	11	22
1	B	234/247 (95%)	214 (92%)	20 (8%)	10	21
1	C	236/247 (96%)	217 (92%)	19 (8%)	11	23
1	D	240/247 (97%)	223 (93%)	17 (7%)	14	29
All	All	941/988 (95%)	866 (92%)	75 (8%)	12	24

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	48	ASN
1	A	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	66	THR
1	A	76	PHE
1	A	87	GLU
1	A	110	LYS
1	A	117	PHE
1	A	159	SER
1	A	175	ASP
1	A	198	MET
1	A	205	LEU
1	A	211	ARG
1	A	213	LYS
1	A	232	ARG
1	A	243	ARG
1	A	306	THR
1	A	310	ARG
1	A	320	ILE
1	B	7	LEU
1	B	48	ASN
1	B	54	VAL
1	B	62	HIS
1	B	63	ARG
1	B	66	THR
1	B	70	THR
1	B	76	PHE
1	B	198	MET
1	B	205	LEU
1	B	210	GLU
1	B	211	ARG
1	B	222	GLU
1	B	252	ARG
1	B	267	LEU
1	B	279	LYS
1	B	286	ILE
1	B	306	THR
1	B	310	ARG
1	B	319	SER
1	C	1	MET
1	C	3	ARG
1	C	7	LEU
1	C	22	SER
1	C	48	ASN
1	C	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	63	ARG
1	C	66	THR
1	C	82	GLN
1	C	105	SER
1	C	117	PHE
1	C	175	ASP
1	C	205	LEU
1	C	215	HIS
1	C	267	LEU
1	C	279	LYS
1	C	288	ASN
1	C	310	ARG
1	C	319	SER
1	D	3	ARG
1	D	7	LEU
1	D	48	ASN
1	D	54	VAL
1	D	62	HIS
1	D	63	ARG
1	D	66	THR
1	D	83	LYS
1	D	91	LYS
1	D	205	LEU
1	D	267	LEU
1	D	270	ARG
1	D	306	THR
1	D	307	ILE
1	D	310	ARG
1	D	319	SER
1	D	320	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	235	GLN
1	B	62	HIS
1	B	235	GLN
1	C	62	HIS
1	C	82	GLN
1	C	235	GLN
1	C	288	ASN
1	C	290	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	62	HIS
1	D	199	ASN
1	D	288	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PGA	A	325	-	8,8,8	1.83	1 (12%)	10,11,11	1.63	1 (10%)
2	PGA	D	325	-	8,8,8	1.89	1 (12%)	10,11,11	1.47	1 (10%)
2	PGA	C	325	-	8,8,8	1.82	1 (12%)	10,11,11	2.03	2 (20%)
2	PGA	B	325	-	8,8,8	1.93	1 (12%)	10,11,11	1.32	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	PGA	A	325	-	-	0/6/6/6	-
2	PGA	D	325	-	-	0/6/6/6	-
2	PGA	C	325	-	-	3/6/6/6	-
2	PGA	B	325	-	-	0/6/6/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	325	PGA	O1-C1	4.45	1.36	1.22
2	A	325	PGA	O1-C1	4.45	1.36	1.22
2	B	325	PGA	O1-C1	4.30	1.36	1.22
2	C	325	PGA	O1-C1	4.28	1.36	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	325	PGA	O1P-C2-C1	-5.07	102.89	110.54
2	A	325	PGA	O1P-C2-C1	-4.27	104.11	110.54
2	D	325	PGA	O1P-C2-C1	-3.35	105.48	110.54
2	C	325	PGA	O3P-P-O1P	2.79	114.17	106.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	325	PGA	C2-O1P-P-O3P
2	C	325	PGA	C2-O1P-P-O4P
2	C	325	PGA	C2-O1P-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	319/319 (100%)	-0.70	2 (0%)	89	88	9, 29, 58, 71	0
1	B	319/319 (100%)	-0.69	1 (0%)	94	93	10, 29, 61, 72	0
1	C	319/319 (100%)	-0.67	1 (0%)	94	93	11, 31, 63, 83	0
1	D	319/319 (100%)	-0.86	0	100	100	10, 26, 45, 63	0
All	All	1276/1276 (100%)	-0.73	4 (0%)	94	93	9, 28, 59, 83	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	HIS	2.7
1	C	160	HIS	2.6
1	A	197	ASP	2.1
1	A	210	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PGA	A	325	9/9	0.97	0.10	33,34,37,37	0
2	PGA	C	325	9/9	0.98	0.08	31,33,38,39	0
2	PGA	B	325	9/9	0.99	0.09	28,30,39,40	0
2	PGA	D	325	9/9	0.99	0.09	33,34,39,43	0

6.5 Other polymers (i)

There are no such residues in this entry.