



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:13 AM UTC

PDB ID : 4RC1 / pdb_00004rc1
Title : Structure of the methanofuran/methanopterine biosynthetic enzyme MJ1099 from *Methanocaldococcus jannaschii* with PRPP
Authors : Bobik, T.A.; Morales, E.J.; Cascio, D.; Sawaya, M.R.; Yeates, T.O.; Rasche, M.E.
Deposited on : 2014-09-14
Resolution : 2.40 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

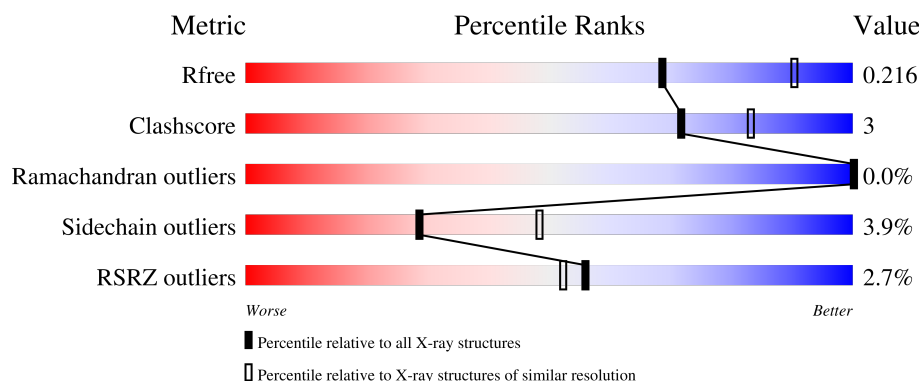
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. 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	242	% 86% 12% .
1	B	242	86% 13% .
1	C	242	84% 12% ..
1	D	242	% 86% 12% .
1	E	242	% 83% 12% ..

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Mol	Chain	Length	Quality of chain
1	F	242	2% 86% 10% • •
1	G	242	7% 85% 11% • •
1	H	242	4% 81% 12% • 5%
1	I	242	7% 86% 10% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16231 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 UPF0264 protein MJ1099.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1814	1155	310	341	8			
1	B	242	Total	C	N	O	S	0	0	0
			1827	1162	315	342	8			
1	C	236	Total	C	N	O	S	0	0	0
			1772	1129	299	336	8			
1	D	242	Total	C	N	O	S	0	0	0
			1827	1162	315	342	8			
1	E	236	Total	C	N	O	S	0	0	0
			1763	1125	296	334	8			
1	F	238	Total	C	N	O	S	0	0	0
			1784	1137	303	336	8			
1	G	236	Total	C	N	O	S	0	0	0
			1772	1129	299	336	8			
1	H	229	Total	C	N	O	S	0	0	0
			1720	1101	286	325	8			
1	I	236	Total	C	N	O	S	0	0	0
			1772	1129	299	336	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q58499
A	-5	HIS	-	expression tag	UNP Q58499
A	-4	HIS	-	expression tag	UNP Q58499
A	-3	HIS	-	expression tag	UNP Q58499
A	-2	HIS	-	expression tag	UNP Q58499
A	-1	HIS	-	expression tag	UNP Q58499
A	0	HIS	-	expression tag	UNP Q58499
B	-6	MET	-	expression tag	UNP Q58499
B	-5	HIS	-	expression tag	UNP Q58499
B	-4	HIS	-	expression tag	UNP Q58499
B	-3	HIS	-	expression tag	UNP Q58499

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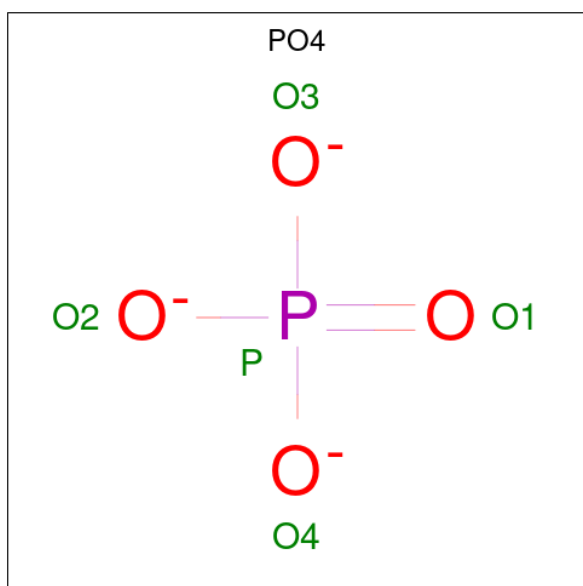
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q58499
B	-1	HIS	-	expression tag	UNP Q58499
B	0	HIS	-	expression tag	UNP Q58499
C	-6	MET	-	expression tag	UNP Q58499
C	-5	HIS	-	expression tag	UNP Q58499
C	-4	HIS	-	expression tag	UNP Q58499
C	-3	HIS	-	expression tag	UNP Q58499
C	-2	HIS	-	expression tag	UNP Q58499
C	-1	HIS	-	expression tag	UNP Q58499
C	0	HIS	-	expression tag	UNP Q58499
D	-6	MET	-	expression tag	UNP Q58499
D	-5	HIS	-	expression tag	UNP Q58499
D	-4	HIS	-	expression tag	UNP Q58499
D	-3	HIS	-	expression tag	UNP Q58499
D	-2	HIS	-	expression tag	UNP Q58499
D	-1	HIS	-	expression tag	UNP Q58499
D	0	HIS	-	expression tag	UNP Q58499
E	-6	MET	-	expression tag	UNP Q58499
E	-5	HIS	-	expression tag	UNP Q58499
E	-4	HIS	-	expression tag	UNP Q58499
E	-3	HIS	-	expression tag	UNP Q58499
E	-2	HIS	-	expression tag	UNP Q58499
E	-1	HIS	-	expression tag	UNP Q58499
E	0	HIS	-	expression tag	UNP Q58499
F	-6	MET	-	expression tag	UNP Q58499
F	-5	HIS	-	expression tag	UNP Q58499
F	-4	HIS	-	expression tag	UNP Q58499
F	-3	HIS	-	expression tag	UNP Q58499
F	-2	HIS	-	expression tag	UNP Q58499
F	-1	HIS	-	expression tag	UNP Q58499
F	0	HIS	-	expression tag	UNP Q58499
G	-6	MET	-	expression tag	UNP Q58499
G	-5	HIS	-	expression tag	UNP Q58499
G	-4	HIS	-	expression tag	UNP Q58499
G	-3	HIS	-	expression tag	UNP Q58499
G	-2	HIS	-	expression tag	UNP Q58499
G	-1	HIS	-	expression tag	UNP Q58499
G	0	HIS	-	expression tag	UNP Q58499
H	-6	MET	-	expression tag	UNP Q58499
H	-5	HIS	-	expression tag	UNP Q58499
H	-4	HIS	-	expression tag	UNP Q58499
H	-3	HIS	-	expression tag	UNP Q58499

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	HIS	-	expression tag	UNP Q58499
H	-1	HIS	-	expression tag	UNP Q58499
H	0	HIS	-	expression tag	UNP Q58499
I	-6	MET	-	expression tag	UNP Q58499
I	-5	HIS	-	expression tag	UNP Q58499
I	-4	HIS	-	expression tag	UNP Q58499
I	-3	HIS	-	expression tag	UNP Q58499
I	-2	HIS	-	expression tag	UNP Q58499
I	-1	HIS	-	expression tag	UNP Q58499
I	0	HIS	-	expression tag	UNP Q58499

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

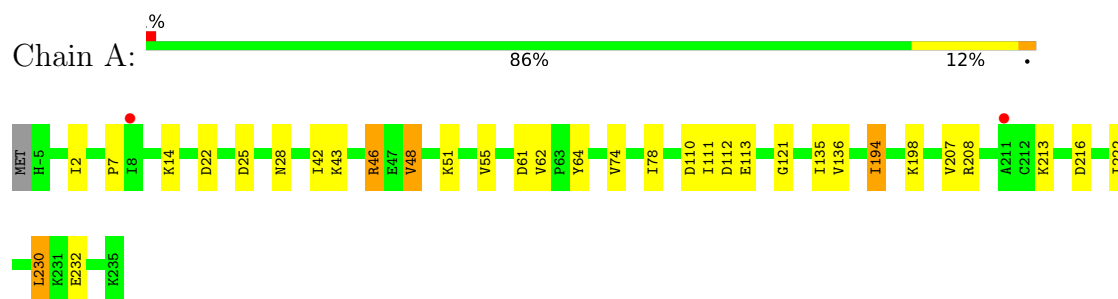
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total 47	O 47	0	0
3	B	38	Total 38	O 38	0	0
3	C	17	Total 17	O 17	0	0
3	D	17	Total 17	O 17	0	0
3	E	16	Total 16	O 16	0	0
3	F	11	Total 11	O 11	0	0
3	G	4	Total 4	O 4	0	0

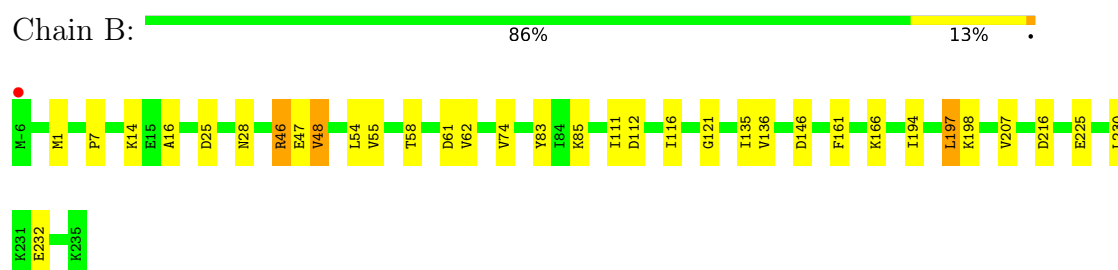
3 Residue-property plots

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.

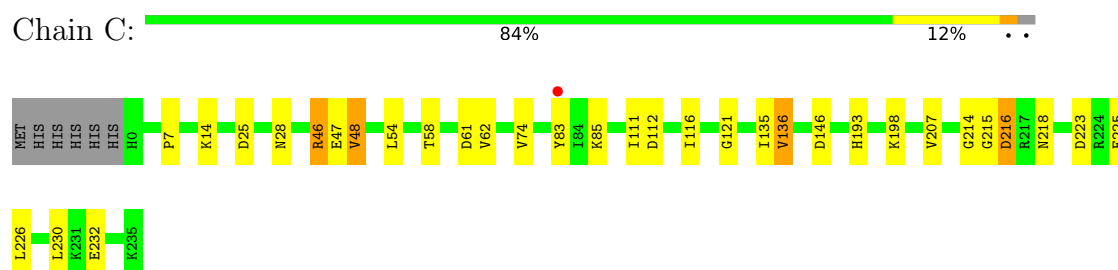
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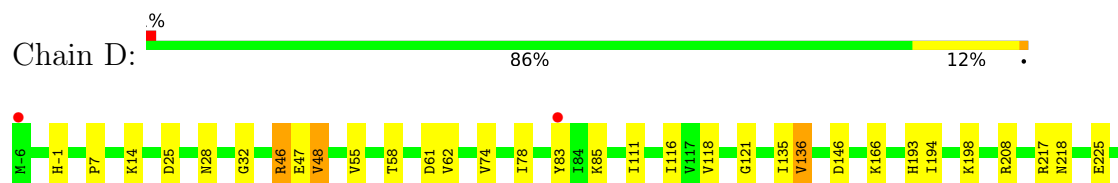
- Molecule 1: UPF0264 protein MJ1099



- Molecule 1: UPF0264 protein MJ1099

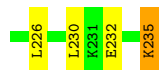
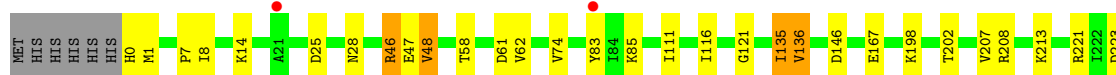
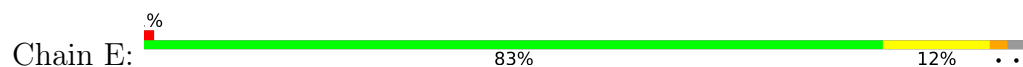


- Molecule 1: UPF0264 protein MJ1099

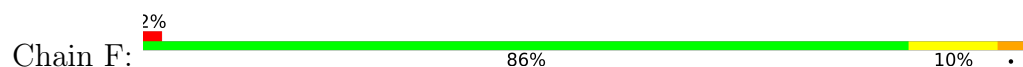




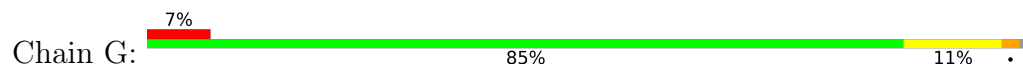
- Molecule 1: UPF0264 protein MJ1099



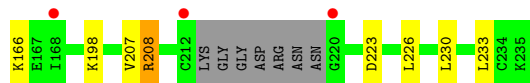
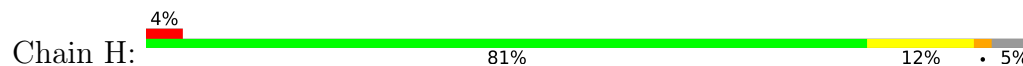
- Molecule 1: UPF0264 protein MJ1099



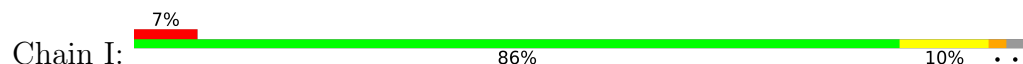
- Molecule 1: UPF0264 protein MJ1099

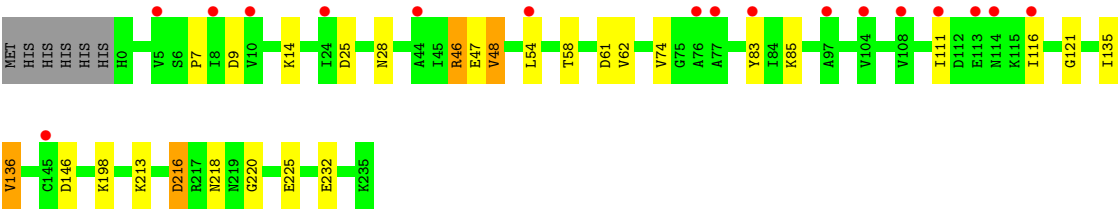


- Molecule 1: UPF0264 protein MJ1099



- Molecule 1: UPF0264 protein MJ1099





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.87Å 153.03Å 132.84Å 90.00° 111.97° 90.00°	Depositor
Resolution (Å)	65.00 – 2.40 65.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (65.00-2.40) 98.4 (65.00-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.40Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.193 , 0.210 0.197 , 0.216	Depositor DCC
R_{free} test set	5118 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16231	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.01	2/1844 (0.1%)	1.50	16/2492 (0.6%)
1	B	0.94	1/1857 (0.1%)	1.42	11/2508 (0.4%)
1	C	0.88	0/1797	1.39	11/2426 (0.5%)
1	D	0.89	1/1857 (0.1%)	1.45	14/2508 (0.6%)
1	E	0.87	0/1788	1.46	9/2415 (0.4%)
1	F	0.90	1/1810 (0.1%)	1.44	11/2444 (0.5%)
1	G	0.86	0/1797	1.42	11/2426 (0.5%)
1	H	0.84	0/1744	1.43	11/2355 (0.5%)
1	I	0.82	0/1797	1.43	11/2426 (0.5%)
All	All	0.89	5/16291 (0.0%)	1.44	105/22000 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	ILE	CA-CB	8.41	1.58	1.54
1	F	41	MET	SD-CE	-7.25	1.61	1.79
1	A	194	ILE	CA-CB	6.80	1.57	1.54
1	D	194	ILE	CA-CB	5.08	1.56	1.54
1	A	64	TYR	CA-C	5.01	1.59	1.53

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	VAL	N-CA-C	12.97	121.08	109.02
1	A	62	VAL	N-CA-C	12.84	120.96	109.02
1	E	62	VAL	N-CA-C	12.72	120.85	109.02
1	I	62	VAL	N-CA-C	12.64	120.77	109.02
1	H	62	VAL	N-CA-C	12.50	120.65	109.02
1	B	62	VAL	N-CA-C	12.35	120.50	109.02
1	D	62	VAL	N-CA-C	12.29	120.45	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	VAL	N-CA-C	11.80	119.99	109.02
1	D	135	ILE	CA-C-N	7.37	124.88	120.24
1	D	135	ILE	C-N-CA	7.37	124.88	120.24
1	B	135	ILE	CA-C-N	6.99	124.64	120.24
1	B	135	ILE	C-N-CA	6.99	124.64	120.24
1	H	135	ILE	CA-C-N	6.78	124.51	120.24
1	H	135	ILE	C-N-CA	6.78	124.51	120.24
1	F	135	ILE	CA-C-N	6.72	124.47	120.24
1	F	135	ILE	C-N-CA	6.72	124.47	120.24
1	A	135	ILE	CA-C-N	6.68	124.45	120.24
1	A	135	ILE	C-N-CA	6.68	124.45	120.24
1	I	220	GLY	N-CA-C	-6.63	105.96	115.64
1	E	61	ASP	N-CA-C	-6.57	97.12	108.56
1	I	135	ILE	CA-C-N	6.57	124.38	120.24
1	I	135	ILE	C-N-CA	6.57	124.38	120.24
1	F	218	ASN	N-CA-C	6.54	120.56	110.42
1	G	135	ILE	CA-C-N	6.48	124.32	120.24
1	G	135	ILE	C-N-CA	6.48	124.32	120.24
1	A	61	ASP	N-CA-C	-6.33	97.54	108.56
1	C	61	ASP	N-CA-C	-6.29	97.62	108.56
1	G	61	ASP	N-CA-C	-6.23	97.73	108.56
1	H	61	ASP	N-CA-C	-6.22	97.73	108.56
1	E	135	ILE	CA-C-N	6.16	124.12	120.24
1	E	135	ILE	C-N-CA	6.16	124.12	120.24
1	C	135	ILE	CA-C-N	6.14	124.11	120.24
1	C	135	ILE	C-N-CA	6.14	124.11	120.24
1	I	9	ASP	N-CA-C	6.14	116.38	108.34
1	F	61	ASP	N-CA-C	-6.10	97.94	108.56
1	E	208	ARG	CA-C-N	6.04	126.81	119.99
1	E	208	ARG	C-N-CA	6.04	126.81	119.99
1	F	1	MET	N-CA-C	5.98	118.40	109.25
1	B	166	LYS	CA-C-N	5.96	128.55	120.44
1	B	166	LYS	C-N-CA	5.96	128.55	120.44
1	D	166	LYS	CA-C-N	5.90	128.11	120.44
1	D	166	LYS	C-N-CA	5.90	128.11	120.44
1	A	42	ILE	CA-C-N	5.83	128.02	120.44
1	A	42	ILE	C-N-CA	5.83	128.02	120.44
1	D	136	VAL	N-CA-CB	5.79	114.15	110.50
1	F	28	ASN	CA-CB-CG	5.76	118.36	112.60
1	H	208	ARG	CA-C-N	5.71	126.42	120.03
1	H	208	ARG	C-N-CA	5.71	126.42	120.03
1	B	28	ASN	CA-CB-CG	5.69	118.29	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	61	ASP	N-CA-C	-5.67	97.32	107.98
1	D	208	ARG	CA-C-N	5.65	126.38	119.99
1	D	208	ARG	C-N-CA	5.65	126.38	119.99
1	D	61	ASP	N-CA-C	-5.63	97.39	107.98
1	B	61	ASP	N-CA-C	-5.62	97.41	107.98
1	A	230	LEU	CA-C-N	5.60	128.05	120.38
1	A	230	LEU	C-N-CA	5.60	128.05	120.38
1	I	9	ASP	CA-C-N	5.59	127.68	120.70
1	I	9	ASP	C-N-CA	5.59	127.68	120.70
1	G	28	ASN	CA-CB-CG	5.53	118.13	112.60
1	F	10	VAL	N-CA-C	5.51	115.71	110.53
1	D	28	ASN	CA-CB-CG	5.50	118.10	112.60
1	G	166	LYS	CA-C-N	5.49	127.58	120.44
1	G	166	LYS	C-N-CA	5.49	127.58	120.44
1	H	136	VAL	N-CA-CB	5.48	113.95	110.50
1	A	208	ARG	CA-C-N	5.47	126.18	119.99
1	A	208	ARG	C-N-CA	5.47	126.18	119.99
1	E	28	ASN	CA-CB-CG	5.47	118.07	112.60
1	I	136	VAL	N-CA-CB	5.42	113.91	110.50
1	H	166	LYS	CA-C-N	5.40	127.46	120.44
1	H	166	LYS	C-N-CA	5.40	127.46	120.44
1	A	28	ASN	CA-CB-CG	5.38	117.98	112.60
1	D	193	HIS	CA-C-N	5.31	125.53	120.43
1	D	193	HIS	C-N-CA	5.31	125.53	120.43
1	A	112	ASP	CA-CB-CG	5.30	117.90	112.60
1	I	28	ASN	CA-CB-CG	5.30	117.90	112.60
1	G	208	ARG	CA-C-N	5.29	125.97	119.99
1	G	208	ARG	C-N-CA	5.29	125.97	119.99
1	H	28	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	198	LYS	CA-C-N	5.26	127.59	120.38
1	A	198	LYS	C-N-CA	5.26	127.59	120.38
1	F	166	LYS	CA-C-N	5.26	127.28	120.44
1	F	166	LYS	C-N-CA	5.26	127.28	120.44
1	C	28	ASN	CA-CB-CG	5.23	117.83	112.60
1	F	136	VAL	N-CA-CB	5.23	113.80	110.50
1	C	215	GLY	CA-C-N	5.20	128.72	121.02
1	C	215	GLY	C-N-CA	5.20	128.72	121.02
1	G	136	VAL	N-CA-CB	5.20	113.77	110.50
1	E	136	VAL	N-CA-CB	5.19	113.77	110.50
1	G	112	ASP	CA-CB-CG	5.17	117.77	112.60
1	B	112	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	193	HIS	CA-C-N	5.15	125.38	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	193	HIS	C-N-CA	5.15	125.38	120.43
1	A	110	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	62	VAL	N-CA-C	5.12	119.94	108.88
1	B	216	ASP	CA-CB-CG	5.12	117.72	112.60
1	E	83	TYR	CB-CA-C	5.10	118.31	110.62
1	A	222	ILE	N-CA-CB	5.08	116.33	110.49
1	H	112	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	136	VAL	N-CA-CB	5.07	113.69	110.50
1	D	32	GLY	CA-C-N	5.07	127.39	120.54
1	D	32	GLY	C-N-CA	5.07	127.39	120.54
1	I	216	ASP	CA-CB-CG	5.05	117.65	112.60
1	B	16	ALA	CA-C-N	5.04	126.92	120.56
1	B	16	ALA	C-N-CA	5.04	126.92	120.56
1	C	112	ASP	CA-CB-CG	5.03	117.62	112.60

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	1814	0	1855	13	0
1	B	1827	0	1875	13	0
1	C	1772	0	1838	12	0
1	D	1827	0	1875	13	0
1	E	1763	0	1825	16	0
1	F	1784	0	1845	13	0
1	G	1772	0	1838	11	0
1	H	1720	0	1789	12	0
1	I	1772	0	1838	9	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	I	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	47	0	0	0	0
3	B	38	0	0	0	0
3	C	17	0	0	0	0
3	D	17	0	0	0	0
3	E	16	0	0	1	0
3	F	11	0	0	0	0
3	G	4	0	0	0	0
All	All	16231	0	16578	109	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 3.

All (109) 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:C:214:GLY:C	1:C:216:ASP:H	2.06	0.61
1:F:83:TYR:CE1	1:F:118:VAL:HG21	2.37	0.60
1:G:7:PRO:HD2	1:G:25:ASP:O	2.02	0.59
1:A:46:ARG:O	1:A:46:ARG:HD3	2.04	0.57
1:E:213:LYS:HG2	1:E:221:ARG:H	1.70	0.57
1:E:223:ASP:HB3	1:E:226:LEU:HD12	1.85	0.57
1:I:7:PRO:HD2	1:I:25:ASP:O	2.05	0.57
1:G:14:LYS:HE2	1:G:48:VAL:HG21	1.88	0.54
1:I:116:ILE:HG23	1:I:146:ASP:HB2	1.89	0.53
1:D:74:VAL:HG13	1:D:111:ILE:HD11	1.91	0.53
1:A:14:LYS:HE2	1:A:48:VAL:HG21	1.91	0.53
1:D:58:THR:HG22	1:D:85:LYS:HD2	1.91	0.53
1:A:7:PRO:HD2	1:A:25:ASP:O	2.09	0.52
1:B:46:ARG:O	1:B:46:ARG:HD3	2.10	0.52
1:E:0:HIS:ND1	1:E:235:LYS:HA	2.24	0.52
1:E:14:LYS:HE2	1:E:48:VAL:HG21	1.90	0.52
1:H:46:ARG:HG3	1:H:80:GLY:O	2.10	0.52
1:D:14:LYS:HE2	1:D:48:VAL:HG21	1.92	0.52
1:F:46:ARG:O	1:F:46:ARG:HD3	2.09	0.52
1:C:46:ARG:O	1:C:46:ARG:HD3	2.09	0.52
1:G:46:ARG:O	1:G:46:ARG:HD3	2.10	0.52
1:E:7:PRO:HD2	1:E:25:ASP:O	2.11	0.51
1:E:46:ARG:O	1:E:46:ARG:HD3	2.10	0.51
1:G:74:VAL:HG13	1:G:111:ILE:HD11	1.91	0.51
1:B:58:THR:HG22	1:B:85:LYS:HD2	1.92	0.50
1:F:194:ILE:HD11	1:F:230:LEU:HD22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:THR:HG22	1:G:85:LYS:HD2	1.93	0.50
1:E:58:THR:HG22	1:E:85:LYS:HD2	1.94	0.50
1:C:74:VAL:HG13	1:C:111:ILE:HD11	1.94	0.50
1:C:207:VAL:HG21	1:C:230:LEU:HD13	1.93	0.50
1:H:58:THR:HG22	1:H:85:LYS:HD2	1.93	0.50
1:D:46:ARG:O	1:D:46:ARG:HD3	2.12	0.50
1:I:121:GLY:HA3	1:I:136:VAL:HG21	1.94	0.49
1:C:14:LYS:HE2	1:C:48:VAL:HG21	1.93	0.49
1:I:14:LYS:HE2	1:I:48:VAL:HG21	1.93	0.49
1:E:74:VAL:HG13	1:E:111:ILE:HD11	1.95	0.49
1:I:46:ARG:O	1:I:46:ARG:HD3	2.12	0.49
1:A:207:VAL:HG21	1:A:230:LEU:HD13	1.95	0.48
1:F:74:VAL:HG13	1:F:111:ILE:HD11	1.95	0.48
1:I:74:VAL:HG13	1:I:111:ILE:HD11	1.94	0.48
1:G:116:ILE:HG23	1:G:146:ASP:HB2	1.94	0.48
1:D:83:TYR:CE1	1:D:118:VAL:HG21	2.49	0.48
1:E:116:ILE:HG23	1:E:146:ASP:HB2	1.95	0.48
1:D:121:GLY:HA3	1:D:136:VAL:HG21	1.96	0.48
1:C:58:THR:HG22	1:C:85:LYS:HD2	1.95	0.48
1:D:-1:HIS:O	1:D:198:LYS:HG2	2.14	0.48
1:B:14:LYS:HE2	1:B:48:VAL:HG21	1.95	0.48
1:G:54:LEU:HD13	1:G:83:TYR:CE1	2.48	0.48
1:F:9:ASP:HA	1:F:41:MET:HE2	1.96	0.47
1:H:14:LYS:HE2	1:H:48:VAL:HG21	1.95	0.47
1:G:121:GLY:HA3	1:G:136:VAL:HG21	1.96	0.47
1:H:116:ILE:HG23	1:H:146:ASP:HB2	1.96	0.47
1:H:121:GLY:HA3	1:H:136:VAL:HG21	1.96	0.47
1:C:54:LEU:HD13	1:C:83:TYR:CE1	2.50	0.47
1:E:207:VAL:HG21	1:E:230:LEU:HD13	1.96	0.47
1:I:58:THR:HG22	1:I:85:LYS:HD2	1.96	0.47
1:F:46:ARG:HD3	1:F:46:ARG:C	2.39	0.47
1:H:207:VAL:HG21	1:H:230:LEU:HD13	1.96	0.47
1:A:74:VAL:HG13	1:A:111:ILE:HD11	1.97	0.47
1:E:1:MET:HG2	1:E:202:THR:O	2.14	0.46
1:E:121:GLY:HA3	1:E:136:VAL:HG21	1.98	0.46
1:E:46:ARG:HD3	1:E:46:ARG:C	2.39	0.46
1:E:0:HIS:CE1	1:E:235:LYS:HG2	2.50	0.46
1:F:116:ILE:HG23	1:F:146:ASP:HB2	1.97	0.46
1:A:121:GLY:HA3	1:A:136:VAL:HG21	1.97	0.46
1:C:121:GLY:HA3	1:C:136:VAL:HG21	1.96	0.46
1:E:0:HIS:HE1	1:E:235:LYS:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:GLY:HA3	1:F:136:VAL:HG21	1.97	0.46
1:B:74:VAL:HG13	1:B:111:ILE:HD11	1.97	0.46
1:B:121:GLY:HA3	1:B:136:VAL:HG21	1.97	0.46
1:F:221:ARG:HH11	1:F:221:ARG:HG2	1.81	0.46
1:C:7:PRO:HD2	1:C:25:ASP:O	2.16	0.46
1:C:116:ILE:HG23	1:C:146:ASP:HB2	1.96	0.45
1:H:74:VAL:HG13	1:H:111:ILE:HD11	1.98	0.45
1:D:116:ILE:HG23	1:D:146:ASP:HB2	1.99	0.45
1:G:46:ARG:HD3	1:G:46:ARG:C	2.41	0.45
1:C:46:ARG:HD3	1:C:46:ARG:C	2.40	0.45
1:H:7:PRO:HD2	1:H:25:ASP:O	2.16	0.45
1:B:7:PRO:HD2	1:B:25:ASP:O	2.18	0.44
1:B:46:ARG:HA	1:B:55:VAL:HG21	2.00	0.44
1:D:46:ARG:HD3	1:D:46:ARG:C	2.42	0.44
1:A:78:ILE:HG21	1:D:78:ILE:HG13	1.99	0.44
1:B:46:ARG:HD3	1:B:46:ARG:C	2.42	0.44
1:D:7:PRO:HD2	1:D:25:ASP:O	2.17	0.44
1:B:1:MET:HE2	1:B:198:LYS:HG3	2.00	0.43
1:G:223:ASP:HB3	1:G:226:LEU:HD12	2.00	0.43
1:H:54:LEU:HD13	1:H:83:TYR:CE1	2.52	0.43
1:H:12:GLU:OE1	1:H:208:ARG:NH2	2.51	0.43
1:I:46:ARG:HD3	1:I:46:ARG:C	2.42	0.43
1:H:223:ASP:HB3	1:H:226:LEU:HD12	2.01	0.43
1:G:208:ARG:NH1	1:G:217:ARG:O	2.52	0.43
1:B:54:LEU:HD13	1:B:83:TYR:CE1	2.54	0.42
1:E:135:ILE:HA	3:E:409:HOH:O	2.19	0.42
1:H:10:VAL:HG13	1:H:48:VAL:HG11	2.01	0.42
1:A:46:ARG:HD3	1:A:46:ARG:C	2.42	0.42
1:B:116:ILE:HG23	1:B:146:ASP:HB2	2.01	0.42
1:B:207:VAL:HG21	1:B:230:LEU:HD13	2.02	0.42
1:I:54:LEU:HD13	1:I:83:TYR:CE1	2.54	0.42
1:D:46:ARG:HA	1:D:55:VAL:HG21	2.02	0.42
1:F:10:VAL:HG13	1:F:48:VAL:HG11	2.02	0.42
1:C:223:ASP:HB3	1:C:226:LEU:HD12	2.03	0.41
1:A:78:ILE:HG13	1:D:78:ILE:HG21	2.01	0.41
1:A:194:ILE:HD11	1:A:230:LEU:HD22	2.03	0.41
1:F:10:VAL:HG23	1:F:41:MET:HE1	2.01	0.41
1:B:161:PHE:HZ	1:B:197:LEU:HD13	1.85	0.41
1:A:2:ILE:HG23	1:A:22:ASP:HB2	2.03	0.41
1:F:11:GLU:HG3	1:F:221:ARG:HH21	1.85	0.41
1:A:113:GLU:HG3	1:F:218:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HA	1:A:55:VAL:HG21	2.02	0.40

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	239/242 (99%)	235 (98%)	4 (2%)	0	100	100
1	B	240/242 (99%)	235 (98%)	5 (2%)	0	100	100
1	C	234/242 (97%)	230 (98%)	4 (2%)	0	100	100
1	D	240/242 (99%)	236 (98%)	4 (2%)	0	100	100
1	E	234/242 (97%)	230 (98%)	4 (2%)	0	100	100
1	F	236/242 (98%)	233 (99%)	3 (1%)	0	100	100
1	G	234/242 (97%)	231 (99%)	3 (1%)	0	100	100
1	H	225/242 (93%)	223 (99%)	2 (1%)	0	100	100
1	I	234/242 (97%)	230 (98%)	3 (1%)	1 (0%)	30	43
All	All	2116/2178 (97%)	2083 (98%)	32 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	213	LYS

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	188/191 (98%)	181 (96%)	7 (4%)	30	51
1	B	190/191 (100%)	184 (97%)	6 (3%)	34	56
1	C	185/191 (97%)	177 (96%)	8 (4%)	26	44
1	D	190/191 (100%)	183 (96%)	7 (4%)	30	51
1	E	183/191 (96%)	175 (96%)	8 (4%)	25	43
1	F	185/191 (97%)	176 (95%)	9 (5%)	22	39
1	G	185/191 (97%)	178 (96%)	7 (4%)	29	49
1	H	180/191 (94%)	175 (97%)	5 (3%)	38	60
1	I	185/191 (97%)	177 (96%)	8 (4%)	26	44
All	All	1671/1719 (97%)	1606 (96%)	65 (4%)	28	48

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

Mol	Chain	Res	Type
1	A	43	LYS
1	A	46	ARG
1	A	48	VAL
1	A	51	LYS
1	A	213	LYS
1	A	216	ASP
1	A	232	GLU
1	B	46	ARG
1	B	47	GLU
1	B	48	VAL
1	B	197	LEU
1	B	225	GLU
1	B	232	GLU
1	C	46	ARG
1	C	47	GLU
1	C	48	VAL
1	C	198	LYS
1	C	216	ASP
1	C	218	ASN
1	C	225	GLU
1	C	232	GLU
1	D	46	ARG
1	D	47	GLU

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Mol	Chain	Res	Type
1	D	48	VAL
1	D	217	ARG
1	D	218	ASN
1	D	225	GLU
1	D	232	GLU
1	E	8	ILE
1	E	46	ARG
1	E	47	GLU
1	E	48	VAL
1	E	167	GLU
1	E	198	LYS
1	E	232	GLU
1	E	235	LYS
1	F	0	HIS
1	F	11	GLU
1	F	46	ARG
1	F	47	GLU
1	F	48	VAL
1	F	198	LYS
1	F	217	ARG
1	F	225	GLU
1	F	232	GLU
1	G	46	ARG
1	G	47	GLU
1	G	48	VAL
1	G	159	THR
1	G	198	LYS
1	G	225	GLU
1	G	232	GLU
1	H	46	ARG
1	H	47	GLU
1	H	48	VAL
1	H	198	LYS
1	H	233	LEU
1	I	46	ARG
1	I	47	GLU
1	I	48	VAL
1	I	198	LYS
1	I	216	ASP
1	I	218	ASN
1	I	225	GLU
1	I	232	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-5	HIS
1	A	-1	HIS
1	B	103	ASN
1	B	218	ASN
1	C	103	ASN
1	D	-4	HIS
1	D	-1	HIS
1	D	164	GLN
1	E	219	ASN
1	F	103	ASN
1	F	218	ASN
1	G	0	HIS
1	G	164	GLN
1	H	164	GLN
1	I	103	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	I	301	-	4,4,4	1.35	1 (25%)	6,6,6	0.47	0
2	PO4	F	301	-	4,4,4	1.48	1 (25%)	6,6,6	0.50	0
2	PO4	D	301	-	4,4,4	1.63	2 (50%)	6,6,6	1.11	1 (16%)
2	PO4	B	301	-	4,4,4	2.82	2 (50%)	6,6,6	1.44	1 (16%)
2	PO4	E	301	-	4,4,4	1.56	1 (25%)	6,6,6	0.47	0
2	PO4	C	301	-	4,4,4	1.43	1 (25%)	6,6,6	1.17	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PO4	P-O4	4.92	1.69	1.54
2	E	301	PO4	P-O1	2.92	1.57	1.50
2	F	301	PO4	P-O1	2.68	1.56	1.50
2	B	301	PO4	P-O1	2.65	1.56	1.50
2	I	301	PO4	P-O1	2.49	1.56	1.50
2	D	301	PO4	P-O4	2.27	1.61	1.54
2	D	301	PO4	P-O1	2.23	1.55	1.50
2	C	301	PO4	P-O1	2.16	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	PO4	O4-P-O2	2.32	115.13	107.91
2	B	301	PO4	O4-P-O3	2.10	114.44	107.91

There are no chirality outliers.

There are no torsion outliers.

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

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	241/242 (99%)	-0.38	2 (0%) 82 80	49, 61, 102, 158	0
1	B	242/242 (100%)	-0.25	1 (0%) 88 86	55, 73, 99, 122	0
1	C	236/242 (97%)	-0.17	1 (0%) 88 86	52, 83, 139, 160	0
1	D	242/242 (100%)	-0.04	2 (0%) 82 80	52, 85, 145, 167	0
1	E	236/242 (97%)	0.19	2 (0%) 82 80	62, 96, 163, 189	0
1	F	238/242 (98%)	0.07	6 (2%) 58 54	63, 95, 137, 163	0
1	G	236/242 (97%)	0.63	17 (7%) 21 18	76, 113, 164, 179	0
1	H	229/242 (94%)	0.76	9 (3%) 43 39	102, 140, 187, 201	0
1	I	236/242 (97%)	0.79	17 (7%) 21 18	102, 146, 185, 206	0
All	All	2136/2178 (98%)	0.17	57 (2%) 56 52	49, 96, 167, 206	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	214	GLY	4.5
1	I	83	TYR	4.3
1	I	24	ILE	4.0
1	H	220	GLY	3.9
1	H	212	CYS	3.8
1	F	-2	HIS	3.8
1	A	211	ALA	3.7
1	I	54	LEU	3.7
1	G	230	LEU	3.7
1	G	83	TYR	3.5
1	E	21	ALA	3.1
1	G	148	ALA	3.0
1	I	97	ALA	3.0
1	G	234	CYS	3.0
1	I	111	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	83	TYR	3.0
1	H	88	LEU	2.9
1	E	83	TYR	2.9
1	I	108	VAL	2.8
1	I	116	ILE	2.8
1	I	5	VAL	2.8
1	G	10	VAL	2.7
1	G	217	ARG	2.7
1	G	185	LEU	2.7
1	G	3	LEU	2.7
1	F	219	ASN	2.6
1	G	186	ALA	2.6
1	G	42	ILE	2.6
1	G	150	LEU	2.5
1	C	83	TYR	2.5
1	I	44	ALA	2.5
1	H	168	ILE	2.4
1	G	225	GLU	2.4
1	I	8	ILE	2.4
1	I	76	ALA	2.4
1	D	-6	MET	2.3
1	H	148	ALA	2.3
1	F	216	ASP	2.3
1	I	104	VAL	2.3
1	F	145	CYS	2.3
1	G	72	ALA	2.3
1	G	184	ALA	2.3
1	H	37	ASN	2.3
1	I	114	ASN	2.2
1	H	87	GLY	2.2
1	I	145	CYS	2.2
1	I	77	ALA	2.1
1	G	189	ILE	2.1
1	G	183	CYS	2.1
1	I	113	GLU	2.1
1	I	10	VAL	2.1
1	F	140	ALA	2.1
1	B	-6	MET	2.1
1	H	36	ALA	2.1
1	A	8	ILE	2.1
1	H	63	PRO	2.0
1	G	207	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PO4	I	301	5/5	0.74	0.10	168,169,169,170	0
2	PO4	B	301	5/5	0.81	0.13	60,79,83,85	0
2	PO4	D	301	5/5	0.82	0.10	110,112,113,115	0
2	PO4	F	301	5/5	0.82	0.13	149,152,153,154	0
2	PO4	C	301	5/5	0.82	0.13	115,115,117,122	0
2	PO4	E	301	5/5	0.83	0.12	142,143,144,145	0

6.5 Other polymers [i](#)

There are no such residues in this entry.