



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 1CDD / pdb_00001cdd
Title : STRUCTURES OF APO AND COMPLEXED ESCHERICHIA COLI
GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE
Authors : Almassy, R.J.; Janson, C.A.; Kan, C.-C.; Hostomska, Z.
Deposited on : 1992-05-15
Resolution : 2.80 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

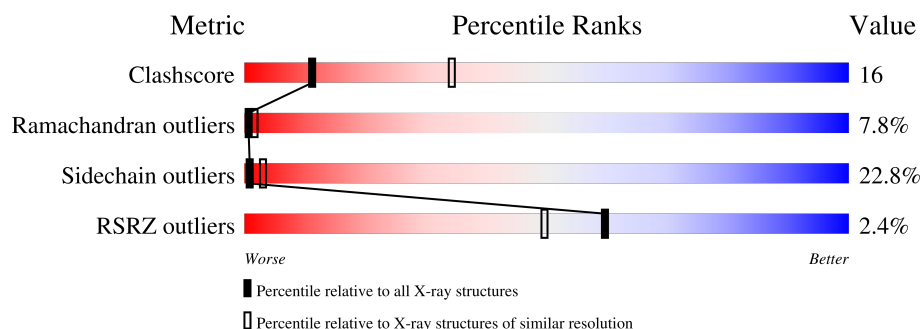
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	212	
1	B	212	

2 Entry composition [i](#)

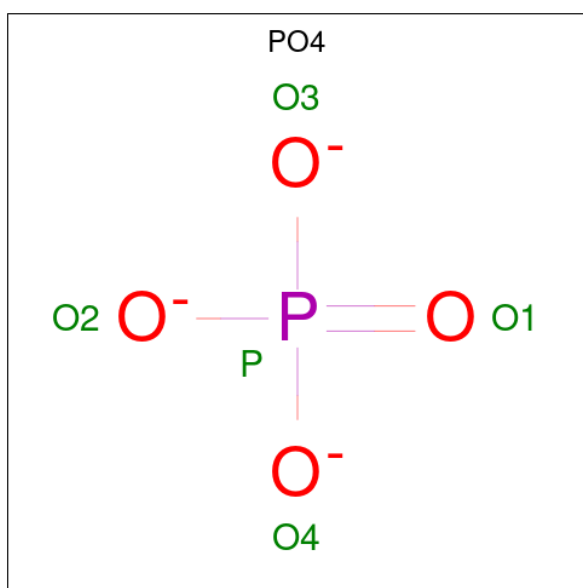
There are 2 unique types of molecules in this entry. The entry contains 2918 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHORIBOSYL-GLYCINAMIDE FORMYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1454	921	255	273	5			
1	B	189	Total	C	N	O	S	0	0	0
			1454	921	255	273	5			

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

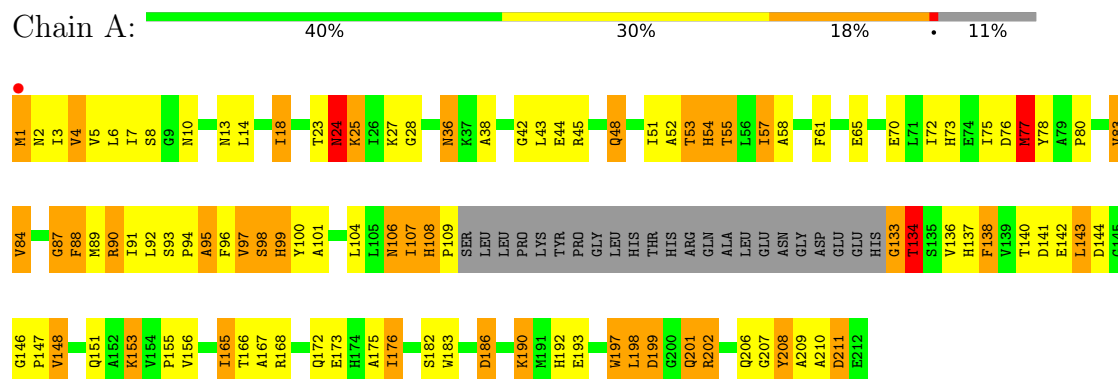


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

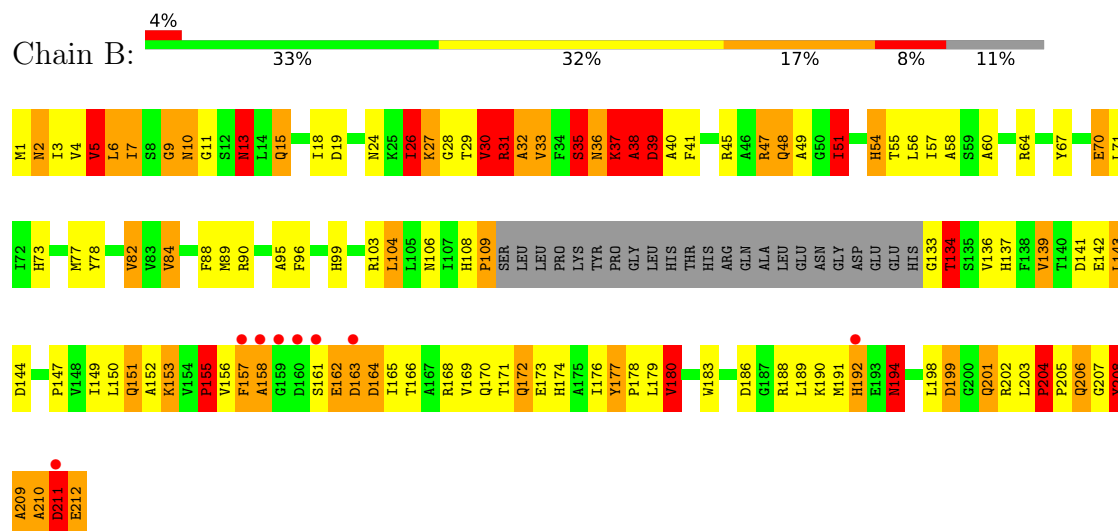
3 Residue-property plots

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.

• Molecule 1: PHOSPHORIBOSYL-GLYCINAMIDE FORMYLTRANSFERASE



• Molecule 1: PHOSPHORIBOSYL-GLYCINAMIDE FORMYLTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	140.90Å 97.60Å 102.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80 80.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 86.9 (80.23-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.82Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.225 , (Not available) 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 79.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2918	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.40	12/1485 (0.8%)	2.36	91/2017 (4.5%)
1	B	1.47	15/1485 (1.0%)	2.66	124/2017 (6.1%)
All	All	1.44	27/2970 (0.9%)	2.51	215/4034 (5.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
1	B	1	1
All	All	2	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	ILE	CA-CB	9.54	1.66	1.54
1	A	148	VAL	CA-CB	9.35	1.66	1.54
1	B	30	VAL	CA-CB	8.79	1.63	1.53
1	B	5	VAL	CA-CB	8.22	1.64	1.54
1	A	176	ILE	CA-CB	7.26	1.64	1.54
1	A	99	HIS	CD2-NE2	-6.94	1.30	1.37
1	B	73	HIS	CD2-NE2	-6.87	1.30	1.37
1	B	180	VAL	CA-CB	6.79	1.63	1.54
1	B	99	HIS	CD2-NE2	-6.58	1.30	1.37
1	B	54	HIS	CD2-NE2	-6.50	1.30	1.37
1	A	54	HIS	CD2-NE2	-6.27	1.30	1.37
1	A	73	HIS	CD2-NE2	-6.26	1.30	1.37
1	A	192	HIS	CD2-NE2	-5.94	1.31	1.37
1	A	84	VAL	CA-CB	5.84	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	VAL	CA-CB	5.81	1.61	1.54
1	B	9	GLY	CA-C	5.77	1.60	1.51
1	B	109	PRO	CA-C	5.69	1.59	1.52
1	B	51	ILE	CA-CB	5.59	1.62	1.54
1	B	210	ALA	N-CA	5.47	1.53	1.46
1	A	108	HIS	CD2-NE2	-5.44	1.31	1.37
1	B	192	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	137	HIS	CD2-NE2	-5.41	1.31	1.37
1	A	73	HIS	CG-ND1	-5.37	1.32	1.38
1	A	53	THR	CA-CB	-5.33	1.44	1.53
1	B	174	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	167	ALA	CA-CB	-5.06	1.45	1.53
1	B	147	PRO	CA-CB	-5.01	1.46	1.53

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	GLU	CB-CA-C	18.43	145.11	110.10
1	B	109	PRO	N-CA-C	14.36	133.60	111.34
1	A	141	ASP	N-CA-C	13.82	130.14	112.03
1	A	36	ASN	OD1-CG-ND2	-13.71	108.89	122.60
1	B	209	ALA	N-CA-C	12.67	137.78	110.80
1	B	210	ALA	N-CA-C	12.30	137.01	110.80
1	B	201	GLN	OE1-CD-NE2	-11.81	110.79	122.60
1	B	133	GLY	CA-C-N	10.96	142.48	121.54
1	B	133	GLY	C-N-CA	10.96	142.48	121.54
1	B	134	THR	CA-CB-OG1	-10.80	93.40	109.60
1	B	163	ASP	CA-CB-CG	10.80	123.40	112.60
1	B	39	ASP	CA-CB-CG	10.38	122.97	112.60
1	B	38	ALA	O-C-N	-10.35	108.83	122.59
1	B	204	PRO	N-CA-C	10.33	123.30	110.70
1	B	206	GLN	OE1-CD-NE2	-10.08	112.52	122.60
1	A	48	GLN	OE1-CD-NE2	-9.69	112.91	122.60
1	A	61	PHE	N-CA-C	9.64	127.51	114.12
1	A	53	THR	CA-CB-OG1	-9.55	95.27	109.60
1	B	204	PRO	CA-N-CD	-9.45	98.76	112.00
1	B	211	ASP	N-CA-C	9.34	130.68	110.80
1	A	134	THR	N-CA-C	9.27	130.55	110.80
1	A	172	GLN	OE1-CD-NE2	-9.19	113.41	122.60
1	B	170	GLN	OE1-CD-NE2	-9.18	113.42	122.60
1	B	194	ASN	OD1-CG-ND2	-9.16	113.44	122.60
1	A	141	ASP	O-C-N	-9.03	113.00	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ASN	CB-CG-ND2	8.86	129.69	116.40
1	A	18	ILE	CB-CG1-CD1	-8.81	95.29	113.80
1	B	134	THR	CA-CB-CG2	8.78	125.43	110.50
1	A	24	ASN	OD1-CG-ND2	-8.76	113.84	122.60
1	B	172	GLN	OE1-CD-NE2	-8.52	114.08	122.60
1	B	36	ASN	OD1-CG-ND2	-8.47	114.13	122.60
1	B	82	VAL	CB-CA-C	-8.36	97.63	110.50
1	B	89	MET	N-CA-C	8.36	123.22	111.52
1	A	133	GLY	CA-C-N	8.33	137.45	121.54
1	A	133	GLY	C-N-CA	8.33	137.45	121.54
1	B	158	ALA	N-CA-C	8.24	128.35	110.80
1	A	201	GLN	CB-CA-C	-8.11	98.10	110.26
1	B	30	VAL	CA-C-O	8.10	130.52	121.04
1	A	48	GLN	CG-CD-NE2	8.03	128.45	116.40
1	A	201	GLN	OE1-CD-NE2	-8.00	114.61	122.60
1	B	210	ALA	CA-C-O	7.99	131.94	120.51
1	B	95	ALA	N-CA-C	7.92	119.91	111.28
1	B	174	HIS	CA-CB-CG	-7.86	105.94	113.80
1	B	201	GLN	CG-CD-NE2	7.86	128.19	116.40
1	A	209	ALA	N-CA-C	7.86	123.63	107.37
1	B	151	GLN	OE1-CD-NE2	-7.84	114.76	122.60
1	B	2	ASN	OD1-CG-ND2	-7.75	114.85	122.60
1	B	133	GLY	O-C-N	7.72	132.74	122.70
1	B	144	ASP	CA-CB-CG	7.61	120.21	112.60
1	A	106	ASN	OD1-CG-ND2	-7.57	115.03	122.60
1	A	137	HIS	N-CA-C	7.49	120.83	109.23
1	B	39	ASP	CB-CA-C	-7.48	95.53	110.42
1	B	24	ASN	N-CA-C	7.46	121.72	112.47
1	B	7	ILE	CB-CA-C	-7.45	100.90	111.40
1	B	172	GLN	CG-CD-NE2	7.42	127.53	116.40
1	B	19	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	54	HIS	CB-CG-CD2	-7.24	121.79	131.20
1	B	194	ASN	CB-CG-ND2	7.22	127.23	116.40
1	B	39	ASP	N-CA-CB	7.22	122.69	110.49
1	A	4	VAL	O-C-N	-7.10	115.59	123.26
1	B	109	PRO	CA-C-O	7.08	130.80	121.95
1	B	31	ARG	CA-CB-CG	7.01	128.12	114.10
1	A	90	ARG	CB-CG-CD	6.99	127.38	111.30
1	B	56	LEU	O-C-N	-6.96	114.02	122.65
1	A	97	VAL	CA-C-O	6.94	128.16	120.95
1	B	6	LEU	CA-C-N	6.93	129.87	122.11
1	B	6	LEU	C-N-CA	6.93	129.87	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	LYS	CA-CB-CG	-6.82	100.46	114.10
1	B	192	HIS	CB-CG-CD2	-6.82	122.33	131.20
1	B	103	ARG	N-CA-C	-6.81	104.52	114.39
1	B	201	GLN	CB-CG-CD	6.73	124.05	112.60
1	B	4	VAL	CA-C-O	-6.73	113.33	120.39
1	B	108	HIS	CB-CG-CD2	-6.73	122.46	131.20
1	A	57	ILE	N-CA-CB	-6.66	103.08	111.41
1	A	186	ASP	CA-CB-CG	6.64	119.24	112.60
1	B	48	GLN	OE1-CD-NE2	-6.63	115.97	122.60
1	A	134	THR	CA-CB-CG2	-6.60	99.28	110.50
1	A	199	ASP	CA-CB-CG	6.58	119.18	112.60
1	B	13	ASN	OD1-CG-ND2	-6.57	116.03	122.60
1	B	35	SER	O-C-N	-6.57	115.25	123.27
1	B	37	LYS	N-CA-C	6.56	120.30	108.69
1	A	144	ASP	N-CA-C	6.54	124.72	110.80
1	B	54	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	B	70	GLU	CA-C-O	-6.49	113.98	120.80
1	A	108	HIS	CA-C-N	6.46	127.92	119.84
1	A	108	HIS	C-N-CA	6.46	127.92	119.84
1	B	212	GLU	N-CA-C	-6.41	93.05	111.00
1	B	2	ASN	CA-C-O	6.40	129.66	120.51
1	A	38	ALA	N-CA-C	6.39	124.42	110.80
1	A	52	ALA	N-CA-C	6.38	118.33	109.15
1	A	192	HIS	CB-CG-CD2	-6.37	122.92	131.20
1	B	203	LEU	N-CA-C	6.35	123.84	109.81
1	B	141	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	73	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	A	73	HIS	CA-CB-CG	-6.24	107.56	113.80
1	B	15	GLN	CB-CA-C	-6.22	100.41	110.74
1	A	13	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	B	82	VAL	N-CA-CB	6.18	121.58	111.44
1	B	143	LEU	N-CA-CB	-6.18	100.37	110.14
1	B	210	ALA	CA-C-N	6.17	133.33	121.54
1	B	210	ALA	C-N-CA	6.17	133.33	121.54
1	A	96	PHE	CA-CB-CG	-6.15	107.65	113.80
1	B	183	TRP	CG-CD2-CE3	6.15	140.05	133.90
1	A	61	PHE	CA-CB-CG	-6.15	107.65	113.80
1	A	53	THR	CA-CB-CG2	6.14	120.94	110.50
1	A	65	GLU	CB-CG-CD	6.10	122.98	112.60
1	B	32	ALA	CB-CA-C	-6.09	98.30	110.42
1	A	92	LEU	N-CA-C	6.07	119.06	110.50
1	A	106	ASN	CB-CG-ND2	6.05	125.47	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	MET	O-C-N	-6.04	113.33	123.00
1	A	202	ARG	CB-CG-CD	-6.03	97.43	111.30
1	A	172	GLN	CG-CD-NE2	6.02	125.43	116.40
1	B	171	THR	CA-CB-OG1	-6.02	100.58	109.60
1	A	104	LEU	N-CA-C	6.00	117.98	108.67
1	A	24	ASN	N-CA-C	6.00	123.58	110.80
1	B	88	PHE	O-C-N	-5.99	114.90	122.27
1	A	134	THR	O-C-N	5.95	130.51	122.59
1	A	201	GLN	N-CA-C	5.94	118.32	109.59
1	B	163	ASP	N-CA-C	-5.93	98.16	110.80
1	B	64	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	B	134	THR	N-CA-C	5.89	123.34	110.80
1	B	162	GLU	O-C-N	5.89	130.42	122.59
1	B	106	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	A	165	ILE	CB-CA-C	-5.87	104.30	111.87
1	A	77	MET	CA-CB-CG	5.87	125.83	114.10
1	B	134	THR	CA-C-O	5.87	128.90	120.51
1	A	97	VAL	N-CA-C	5.84	116.58	110.62
1	B	157	PHE	O-C-N	5.84	130.36	122.59
1	A	133	GLY	O-C-N	5.83	130.28	122.70
1	A	201	GLN	N-CA-CB	5.83	118.68	109.71
1	A	51	ILE	N-CA-C	5.82	117.12	109.21
1	A	137	HIS	CA-CB-CG	5.81	119.61	113.80
1	A	151	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	B	201	GLN	N-CA-C	5.80	118.67	109.50
1	A	138	PHE	N-CA-C	5.79	117.48	109.15
1	B	84	VAL	CA-C-O	5.78	126.72	120.53
1	B	204	PRO	CB-CA-C	5.75	117.94	110.92
1	A	137	HIS	O-C-N	-5.75	116.60	123.27
1	B	137	HIS	CB-CG-CD2	-5.74	123.74	131.20
1	B	13	ASN	CA-C-N	5.72	127.88	120.44
1	B	13	ASN	C-N-CA	5.72	127.88	120.44
1	B	162	GLU	CA-C-O	5.69	128.65	120.51
1	B	7	ILE	O-C-N	-5.69	116.76	122.67
1	A	7	ILE	CB-CA-C	-5.66	102.44	110.82
1	B	212	GLU	CB-CG-CD	5.63	122.17	112.60
1	A	143	LEU	CA-C-O	5.63	127.05	121.20
1	B	96	PHE	O-C-N	5.62	127.88	122.03
1	B	137	HIS	CE1-NE2-CD2	5.61	114.61	109.00
1	A	138	PHE	O-C-N	-5.60	115.20	122.77
1	B	6	LEU	O-C-N	-5.59	116.64	122.96
1	B	204	PRO	N-CA-CB	-5.56	97.69	103.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	PRO	CB-CA-C	5.56	116.46	111.40
1	B	37	LYS	CA-CB-CG	-5.55	102.99	114.10
1	A	155	PRO	N-CA-C	5.52	119.14	110.80
1	A	211	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	54	HIS	O-C-N	-5.50	117.14	123.42
1	A	70	GLU	N-CA-C	5.50	116.95	111.07
1	B	9	GLY	N-CA-C	5.49	126.20	113.18
1	B	88	PHE	CA-CB-CG	5.49	119.28	113.80
1	B	162	GLU	N-CA-C	5.49	122.48	110.80
1	B	162	GLU	CA-C-N	5.48	132.00	121.54
1	B	162	GLU	C-N-CA	5.48	132.00	121.54
1	A	52	ALA	CB-CA-C	-5.47	102.35	110.67
1	B	106	ASN	CB-CG-ND2	5.46	124.59	116.40
1	B	9	GLY	O-C-N	-5.46	115.61	122.70
1	A	176	ILE	CB-CA-C	5.45	119.06	111.92
1	A	2	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	B	33	VAL	N-CA-C	5.43	115.78	108.17
1	B	10	ASN	CA-C-O	-5.43	112.75	120.51
1	B	33	VAL	O-C-N	-5.43	117.48	123.18
1	B	108	HIS	CB-CG-ND1	5.39	130.79	122.70
1	A	53	THR	N-CA-CB	-5.38	102.66	110.36
1	B	204	PRO	CA-CB-CG	-5.38	94.28	104.50
1	B	192	HIS	CB-CG-ND1	5.38	130.77	122.70
1	A	36	ASN	N-CA-C	-5.38	106.67	113.18
1	B	209	ALA	N-CA-CB	-5.38	101.40	110.49
1	A	88	PHE	O-C-N	-5.37	115.83	122.82
1	B	5	VAL	N-CA-C	5.34	115.55	107.75
1	B	48	GLN	CG-CD-NE2	5.34	124.41	116.40
1	A	57	ILE	CB-CA-C	5.33	118.77	111.31
1	A	76	ASP	N-CA-C	5.31	117.98	111.82
1	B	208	TYR	O-C-N	-5.31	115.53	122.59
1	B	139	VAL	CB-CA-C	-5.30	104.25	111.15
1	B	155	PRO	N-CA-C	5.30	119.53	111.15
1	A	3	ILE	O-C-N	-5.26	116.72	122.83
1	B	2	ASN	N-CA-C	5.26	122.01	110.80
1	B	88	PHE	CA-C-O	-5.25	113.93	119.97
1	A	94	PRO	N-CA-C	-5.25	101.61	110.21
1	B	33	VAL	CA-CB-CG2	-5.23	101.50	110.40
1	A	10	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	148	VAL	CA-CB-CG2	5.22	119.28	110.40
1	B	13	ASN	CA-CB-CG	-5.21	107.39	112.60
1	B	109	PRO	N-CA-CB	-5.20	98.50	103.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ILE	CA-C-O	-5.19	116.83	121.09
1	A	1	MET	CB-CG-SD	5.18	128.25	112.70
1	A	166	THR	CA-CB-OG1	-5.16	101.86	109.60
1	A	134	THR	CA-CB-OG1	5.15	117.33	109.60
1	A	2	ASN	N-CA-C	5.14	117.08	108.23
1	B	210	ALA	O-C-N	5.14	129.43	122.59
1	A	55	THR	CA-C-O	5.14	125.69	120.24
1	B	19	ASP	O-C-N	-5.13	116.21	122.22
1	B	157	PHE	CA-C-N	5.12	131.32	121.54
1	B	157	PHE	C-N-CA	5.12	131.32	121.54
1	B	186	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	197	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	A	87	GLY	O-C-N	-5.07	116.03	122.32
1	A	192	HIS	CB-CG-ND1	5.07	130.30	122.70
1	A	197	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	A	153	LYS	CA-CB-CG	5.05	124.20	114.10
1	B	31	ARG	N-CA-CB	-5.04	101.97	110.49
1	A	175	ALA	CA-C-O	5.03	125.10	119.41
1	A	182	SER	CB-CA-C	-5.03	103.21	110.96
1	B	137	HIS	ND1-CE1-NE2	-5.03	103.38	108.40
1	B	56	LEU	N-CA-CB	-5.00	102.25	110.11
1	B	89	MET	CA-C-O	5.00	127.50	121.65

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	212	GLU	CA
1	B	212	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	204	PRO	Peptide

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	1454	0	1434	44	0
1	B	1454	0	1434	57	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
All	All	2918	0	2868	94	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 16.

All (94) 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:42:GLY:HA2	1:A:45:ARG:HG3	1.52	0.89
1:B:15:GLN:HG2	1:B:45:ARG:HD3	1.65	0.79
1:A:138:PHE:HB2	1:A:147:PRO:HG2	1.69	0.75
1:A:43:LEU:HD22	1:A:53:THR:HG23	1.70	0.73
1:A:54:HIS:HD2	1:B:54:HIS:HD2	1.36	0.73
1:B:33:VAL:HG23	1:B:51:ILE:HD11	1.71	0.73
1:B:10:ASN:HD21	1:B:45:ARG:HH21	1.39	0.70
1:B:54:HIS:HE1	1:B:78:TYR:OH	1.75	0.69
1:B:1:MET:HA	1:B:28:GLY:HA2	1.75	0.68
1:B:10:ASN:HD21	1:B:45:ARG:NH2	1.92	0.67
1:B:13:ASN:HD21	1:B:173:GLU:HB3	1.60	0.66
1:A:54:HIS:HE1	1:A:78:TYR:OH	1.83	0.62
1:B:3:ILE:HD11	1:B:26:ILE:HD11	1.82	0.61
1:B:155:PRO:HB2	1:B:168:ARG:HH12	1.65	0.61
1:B:134:THR:HG23	1:B:176:ILE:HD11	1.83	0.61
1:B:30:VAL:HG22	1:B:51:ILE:HD13	1.84	0.60
1:A:8:SER:HB2	1:A:87:GLY:O	2.03	0.59
1:A:134:THR:HG21	1:A:173:GLU:HG2	1.86	0.58
1:B:150:LEU:HD22	1:B:176:ILE:HB	1.85	0.57
1:B:136:VAL:HG11	1:B:180:VAL:HG11	1.87	0.56
1:B:5:VAL:HG13	1:B:33:VAL:HG22	1.88	0.56
1:A:4:VAL:HG21	1:A:75:ILE:HG23	1.88	0.56
1:A:43:LEU:HD22	1:A:53:THR:CG2	2.36	0.56
1:B:155:PRO:HB2	1:B:168:ARG:NH1	2.21	0.55
1:B:10:ASN:ND2	1:B:45:ARG:HH21	2.03	0.55
1:B:1:MET:HA	1:B:28:GLY:CA	2.36	0.54
1:A:95:ALA:O	1:A:99:HIS:HB2	2.07	0.54
1:B:7:ILE:O	1:B:35:SER:HA	2.08	0.53
1:A:138:PHE:O	1:A:146:GLY:HA3	2.09	0.53
1:B:104:LEU:HD13	1:B:139:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ARG:HD2	1:B:199:ASP:OD1	2.10	0.52
1:A:106:ASN:ND2	1:A:107:ILE:H	2.08	0.52
1:A:44:GLU:HB2	1:B:47:ARG:HH11	1.75	0.52
1:A:134:THR:CG2	1:A:173:GLU:HG2	2.40	0.51
1:A:44:GLU:HB2	1:B:47:ARG:NH1	2.26	0.51
1:A:156:VAL:HG23	1:A:165:ILE:HD11	1.91	0.51
1:B:153:LYS:O	1:B:153:LYS:HD2	2.11	0.50
1:A:88:PHE:CE2	1:A:90:ARG:HB3	2.46	0.50
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.93	0.50
1:A:83:VAL:HG11	1:A:100:TYR:CD1	2.46	0.49
1:B:150:LEU:CD2	1:B:176:ILE:HB	2.42	0.49
1:B:57:ILE:HG13	1:B:57:ILE:O	2.10	0.49
1:B:11:GLY:H	1:B:45:ARG:HE	1.61	0.49
1:A:54:HIS:HD2	1:B:54:HIS:CD2	2.25	0.49
1:B:204:PRO:O	1:B:206:GLN:N	2.47	0.48
1:A:77:MET:HE1	1:B:70:GLU:CD	2.38	0.48
1:A:197:TRP:CZ3	1:A:202:ARG:HB2	2.49	0.48
1:B:166:THR:O	1:B:169:VAL:HG22	2.14	0.48
1:B:188:ARG:O	1:B:198:LEU:HD12	2.13	0.48
1:B:2:ASN:HD21	1:B:31:ARG:HH11	1.61	0.48
1:A:106:ASN:HD22	1:A:107:ILE:H	1.61	0.48
1:B:149:ILE:HG21	1:B:189:LEU:HD21	1.96	0.48
1:B:10:ASN:HA	1:B:41:PHE:HB3	1.95	0.48
1:A:198:LEU:HB3	1:A:199:ASP:H	1.58	0.48
1:A:1:MET:HA	1:A:28:GLY:HA2	1.96	0.47
1:A:97:VAL:HG23	1:A:98:SER:N	2.28	0.47
1:B:7:ILE:HG13	1:B:35:SER:HB2	1.97	0.47
1:B:67:TYR:CD1	1:B:67:TYR:C	2.93	0.47
1:B:37:LYS:HD3	1:B:37:LYS:HA	1.60	0.46
1:A:4:VAL:HG13	1:A:80:PRO:HB3	1.98	0.46
1:A:6:LEU:HD13	1:A:83:VAL:HG23	1.99	0.45
1:B:190:LYS:HB3	1:B:190:LYS:HE2	1.70	0.45
1:A:93:SER:O	1:A:97:VAL:HG22	2.17	0.45
1:A:72:ILE:HG23	1:A:100:TYR:OH	2.17	0.45
1:B:172:GLN:O	1:B:176:ILE:HG12	2.18	0.44
1:B:134:THR:HG22	1:B:152:ALA:HB3	1.99	0.44
1:A:77:MET:HE3	1:A:77:MET:HB3	1.76	0.43
1:B:191:MET:HE3	1:B:194:ASN:HA	1.99	0.43
1:A:18:ILE:HG21	1:A:18:ILE:HD13	1.80	0.43
1:A:54:HIS:CD2	1:B:54:HIS:HD2	2.25	0.43
1:A:72:ILE:HG12	1:A:100:TYR:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:HIS:HA	1:A:109:PRO:HD3	1.74	0.43
1:A:91:ILE:HD13	1:A:91:ILE:HG21	1.70	0.43
1:B:36:ASN:ND2	1:B:90:ARG:HB2	2.34	0.43
1:B:199:ASP:HB2	1:B:211:ASP:CG	2.44	0.43
1:A:183:TRP:CE3	1:A:198:LEU:HD11	2.54	0.42
1:B:15:GLN:O	1:B:18:ILE:HG12	2.19	0.42
1:A:183:TRP:CZ3	1:A:198:LEU:HD11	2.54	0.42
1:A:108:HIS:O	1:A:134:THR:HA	2.19	0.42
1:B:202:ARG:C	1:B:204:PRO:HD2	2.45	0.42
1:A:77:MET:HE1	1:B:70:GLU:OE1	2.18	0.42
1:A:197:TRP:CD1	1:A:197:TRP:N	2.87	0.42
1:A:1:MET:HA	1:A:28:GLY:CA	2.49	0.42
1:B:15:GLN:HG2	1:B:45:ARG:HH11	1.85	0.42
1:B:18:ILE:HD12	1:B:49:ALA:HB2	2.00	0.42
1:B:15:GLN:CG	1:B:45:ARG:HH11	2.34	0.41
1:B:67:TYR:HE1	1:B:71:LEU:HD22	1.85	0.41
1:B:37:LYS:C	1:B:38:ALA:O	2.63	0.41
1:B:77:MET:HE2	1:B:78:TYR:CE2	2.56	0.41
1:A:190:LYS:HB2	1:A:190:LYS:HE3	1.89	0.40
1:A:107:ILE:HG13	1:A:108:HIS:N	2.36	0.40
1:A:207:GLY:O	1:A:208:TYR:HB3	2.21	0.40
1:B:58:ALA:C	1:B:60:ALA:H	2.29	0.40
1:B:149:ILE:HD13	1:B:189:LEU:HD21	2.03	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	187/212 (88%)	158 (84%)	19 (10%)	10 (5%)	1	5
1	B	187/212 (88%)	145 (78%)	23 (12%)	19 (10%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	374/424 (88%)	303 (81%)	42 (11%)	29 (8%)	1 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	THR
1	A	210	ALA
1	B	32	ALA
1	B	38	ALA
1	B	40	ALA
1	B	158	ALA
1	B	204	PRO
1	B	207	GLY
1	B	209	ALA
1	B	211	ASP
1	A	95	ALA
1	A	101	ALA
1	A	186	ASP
1	A	193	GLU
1	A	208	TYR
1	B	163	ASP
1	B	134	THR
1	B	162	GLU
1	B	210	ALA
1	A	24	ASN
1	B	39	ASP
1	B	208	TYR
1	B	27	LYS
1	B	31	ARG
1	B	164	ASP
1	B	199	ASP
1	A	58	ALA
1	B	9	GLY
1	A	133	GLY

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	151/171 (88%)	121 (80%)	30 (20%)	1	5
1	B	151/171 (88%)	112 (74%)	39 (26%)	0	2
All	All	302/342 (88%)	233 (77%)	69 (23%)	1	3

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	14	LEU
1	A	23	THR
1	A	24	ASN
1	A	25	LYS
1	A	27	LYS
1	A	36	ASN
1	A	48	GLN
1	A	55	THR
1	A	57	ILE
1	A	77	MET
1	A	83	VAL
1	A	84	VAL
1	A	89	MET
1	A	98	SER
1	A	107	ILE
1	A	134	THR
1	A	136	VAL
1	A	140	THR
1	A	142	GLU
1	A	143	LEU
1	A	148	VAL
1	A	153	LYS
1	A	168	ARG
1	A	176	ILE
1	A	190	LYS
1	A	198	LEU
1	A	201	GLN
1	A	206	GLN
1	A	211	ASP
1	B	5	VAL
1	B	6	LEU
1	B	13	ASN
1	B	26	ILE

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Mol	Chain	Res	Type
1	B	27	LYS
1	B	29	THR
1	B	30	VAL
1	B	35	SER
1	B	37	LYS
1	B	39	ASP
1	B	47	ARG
1	B	48	GLN
1	B	51	ILE
1	B	55	THR
1	B	82	VAL
1	B	84	VAL
1	B	104	LEU
1	B	109	PRO
1	B	134	THR
1	B	142	GLU
1	B	143	LEU
1	B	151	GLN
1	B	153	LYS
1	B	155	PRO
1	B	156	VAL
1	B	157	PHE
1	B	161	SER
1	B	164	ASP
1	B	165	ILE
1	B	177	TYR
1	B	179	LEU
1	B	180	VAL
1	B	192	HIS
1	B	194	ASN
1	B	201	GLN
1	B	204	PRO
1	B	205	PRO
1	B	208	TYR
1	B	212	GLU

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	2	ASN
1	A	54	HIS
1	A	106	ASN

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Mol	Chain	Res	Type
1	B	2	ASN
1	B	10	ASN
1	B	13	ASN
1	B	54	HIS
1	B	137	HIS
1	B	170	GLN
1	B	174	HIS
1	B	206	GLN

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](#)

2 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	B	221	-	4,4,4	3.03	1 (25%)	6,6,6	1.50	1 (16%)
2	PO4	A	221	-	4,4,4	2.94	1 (25%)	6,6,6	0.67	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	PO4	P-O4	-5.64	1.38	1.54
2	A	221	PO4	P-O4	-5.50	1.38	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	221	PO4	O3-P-O2	2.56	115.86	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 [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	189/212 (89%)	-0.78	1 (0%) 87 82	8, 29, 66, 122	0
1	B	189/212 (89%)	-0.43	8 (4%) 40 32	6, 31, 93, 146	0
All	All	378/424 (89%)	-0.61	9 (2%) 59 49	6, 30, 81, 146	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	GLY	6.0
1	B	158	ALA	4.8
1	B	163	ASP	4.4
1	B	160	ASP	3.4
1	B	211	ASP	2.8
1	A	1	MET	2.6
1	B	192	HIS	2.6
1	B	157	PHE	2.2
1	B	161	SER	2.2

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	B	221	5/5	0.98	0.07	40,42,50,56	0
2	PO4	A	221	5/5	0.99	0.05	29,33,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.