



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:22 AM UTC

PDB ID : 3OZF / pdb_00003ozf
Title : Crystal Structure of Plasmodium falciparum Hypoxanthine-Guanine-Xanthine Phosphoribosyltransferase in complex with hypoxanthine
Authors : Ho, M.; Hazleton, K.Z.; Almo, S.C.; Schramm, V.L.
Deposited on : 2010-09-24
Resolution : 1.94 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

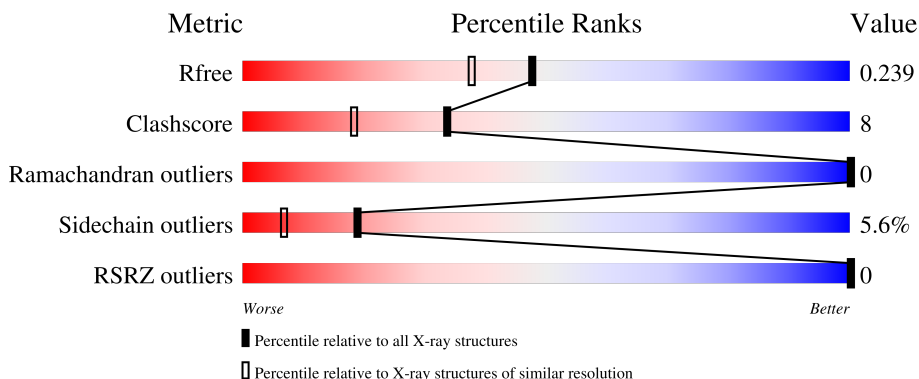
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	250	 77% 15% • 7%
1	B	250	 81% 11% • 6%
1	C	250	 78% 12% • 9%
1	D	250	 76% 12% • 9%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7955 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 Hypoxanthine-guanine-xanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	1	0
			1878	1217	311	340	10			
1	B	234	Total	C	N	O	S	0	0	0
			1882	1220	312	341	9			
1	C	228	Total	C	N	O	S	0	1	0
			1844	1197	304	335	8			
1	D	228	Total	C	N	O	S	0	1	0
			1840	1196	301	335	8			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P20035
A	-17	GLY	-	expression tag	UNP P20035
A	-16	GLY	-	expression tag	UNP P20035
A	-15	SER	-	expression tag	UNP P20035
A	-14	HIS	-	expression tag	UNP P20035
A	-13	HIS	-	expression tag	UNP P20035
A	-12	HIS	-	expression tag	UNP P20035
A	-11	HIS	-	expression tag	UNP P20035
A	-10	HIS	-	expression tag	UNP P20035
A	-9	HIS	-	expression tag	UNP P20035
A	-8	GLY	-	expression tag	UNP P20035
A	-7	GLY	-	expression tag	UNP P20035
A	-6	LEU	-	expression tag	UNP P20035
A	-5	VAL	-	expression tag	UNP P20035
A	-4	PRO	-	expression tag	UNP P20035
A	-3	ARG	-	expression tag	UNP P20035
A	-2	GLY	-	expression tag	UNP P20035
A	-1	SER	-	expression tag	UNP P20035
A	0	HIS	-	expression tag	UNP P20035
B	-18	MET	-	expression tag	UNP P20035
B	-17	GLY	-	expression tag	UNP P20035

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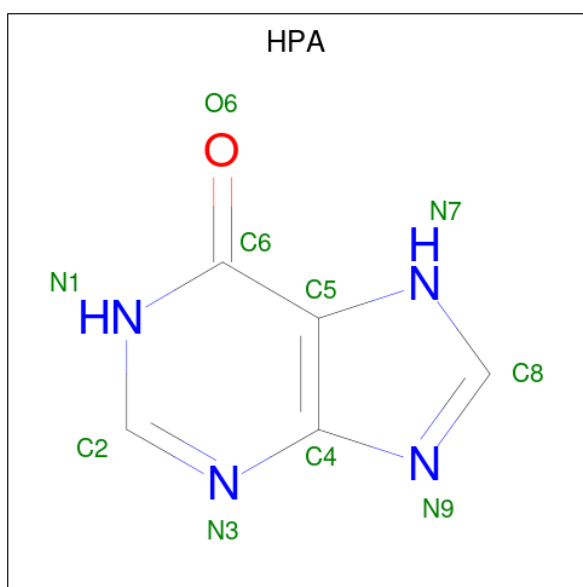
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	GLY	-	expression tag	UNP P20035
B	-15	SER	-	expression tag	UNP P20035
B	-14	HIS	-	expression tag	UNP P20035
B	-13	HIS	-	expression tag	UNP P20035
B	-12	HIS	-	expression tag	UNP P20035
B	-11	HIS	-	expression tag	UNP P20035
B	-10	HIS	-	expression tag	UNP P20035
B	-9	HIS	-	expression tag	UNP P20035
B	-8	GLY	-	expression tag	UNP P20035
B	-7	GLY	-	expression tag	UNP P20035
B	-6	LEU	-	expression tag	UNP P20035
B	-5	VAL	-	expression tag	UNP P20035
B	-4	PRO	-	expression tag	UNP P20035
B	-3	ARG	-	expression tag	UNP P20035
B	-2	GLY	-	expression tag	UNP P20035
B	-1	SER	-	expression tag	UNP P20035
B	0	HIS	-	expression tag	UNP P20035
C	-18	MET	-	expression tag	UNP P20035
C	-17	GLY	-	expression tag	UNP P20035
C	-16	GLY	-	expression tag	UNP P20035
C	-15	SER	-	expression tag	UNP P20035
C	-14	HIS	-	expression tag	UNP P20035
C	-13	HIS	-	expression tag	UNP P20035
C	-12	HIS	-	expression tag	UNP P20035
C	-11	HIS	-	expression tag	UNP P20035
C	-10	HIS	-	expression tag	UNP P20035
C	-9	HIS	-	expression tag	UNP P20035
C	-8	GLY	-	expression tag	UNP P20035
C	-7	GLY	-	expression tag	UNP P20035
C	-6	LEU	-	expression tag	UNP P20035
C	-5	VAL	-	expression tag	UNP P20035
C	-4	PRO	-	expression tag	UNP P20035
C	-3	ARG	-	expression tag	UNP P20035
C	-2	GLY	-	expression tag	UNP P20035
C	-1	SER	-	expression tag	UNP P20035
C	0	HIS	-	expression tag	UNP P20035
D	-18	MET	-	expression tag	UNP P20035
D	-17	GLY	-	expression tag	UNP P20035
D	-16	GLY	-	expression tag	UNP P20035
D	-15	SER	-	expression tag	UNP P20035
D	-14	HIS	-	expression tag	UNP P20035
D	-13	HIS	-	expression tag	UNP P20035

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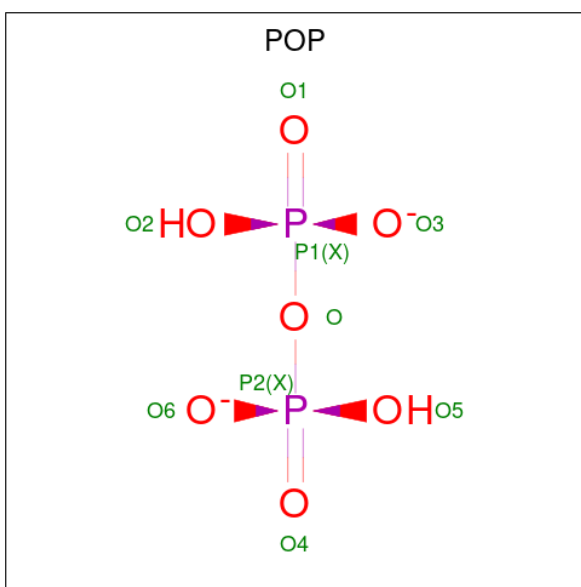
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P20035
D	-11	HIS	-	expression tag	UNP P20035
D	-10	HIS	-	expression tag	UNP P20035
D	-9	HIS	-	expression tag	UNP P20035
D	-8	GLY	-	expression tag	UNP P20035
D	-7	GLY	-	expression tag	UNP P20035
D	-6	LEU	-	expression tag	UNP P20035
D	-5	VAL	-	expression tag	UNP P20035
D	-4	PRO	-	expression tag	UNP P20035
D	-3	ARG	-	expression tag	UNP P20035
D	-2	GLY	-	expression tag	UNP P20035
D	-1	SER	-	expression tag	UNP P20035
D	0	HIS	-	expression tag	UNP P20035

- Molecule 2 is HYPOXANTHINE (CCD ID: HPA) (formula: $C_5H_4N_4O$).



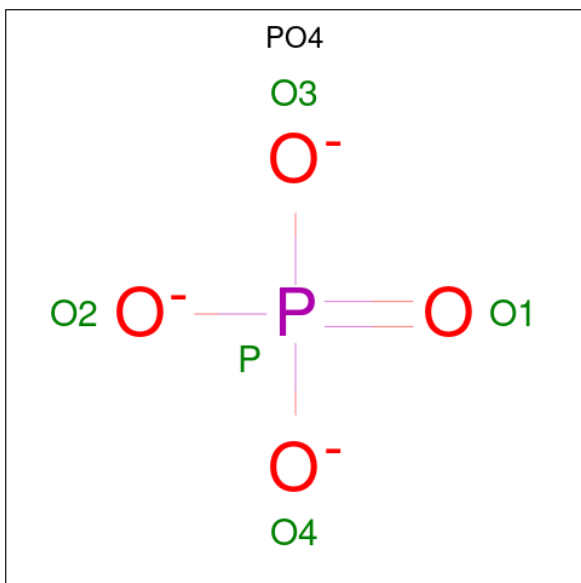
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	4	1		
2	B	1	Total	C	N	O	0	0
			10	5	4	1		
2	C	1	Total	C	N	O	0	0
			10	5	4	1		
2	D	1	Total	C	N	O	0	0
			10	5	4	1		

- Molecule 3 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			9	7	2		
3	B	1	Total	O	P	0	0
			9	7	2		
3	C	1	Total	O	P	0	0
			9	7	2		
3	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0

- Molecule 6 is water.

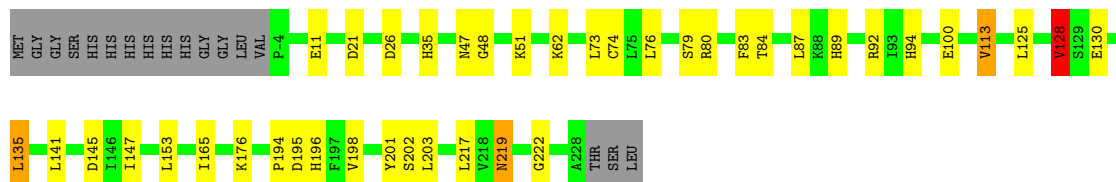
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	94	Total O 94 94	0	0
6	B	97	Total O 97 97	0	0
6	C	110	Total O 110 110	0	0
6	D	108	Total O 108 108	0	0

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.

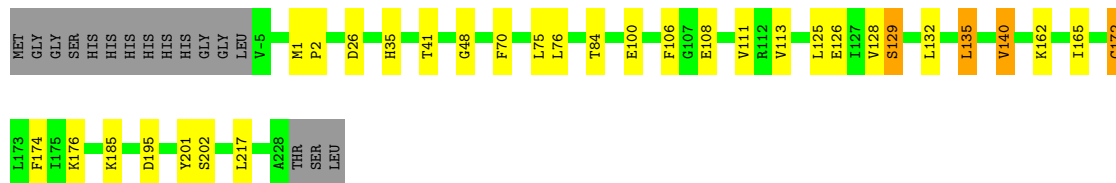
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain A: 



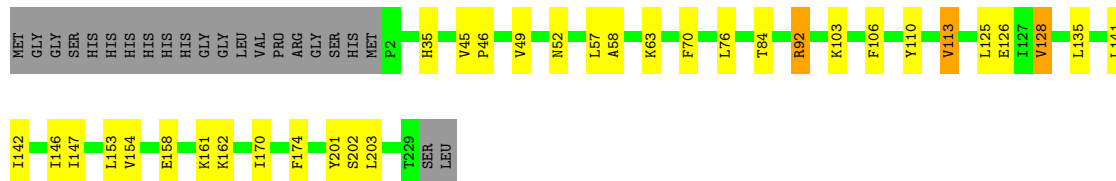
- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain B: 



- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain C: 



- Molecule 1: Hypoxanthine-guanine-xanthine phosphoribosyltransferase

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.03Å 88.91Å 80.37Å 90.00° 117.06° 90.00°	Depositor
Resolution (Å)	35.78 – 1.94 35.78 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.78-1.94) 96.3 (35.78-1.94)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.189 , 0.237 0.189 , 0.239	Depositor DCC
R_{free} test set	3498 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.329 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7955	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% 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, HPA, POP, MG

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	0.82	1/1928 (0.1%)	0.94	2/2603 (0.1%)
1	B	0.83	0/1929	0.96	1/2606 (0.0%)
1	C	0.82	1/1892 (0.1%)	0.91	0/2555
1	D	0.83	0/1888	0.95	1/2551 (0.0%)
All	All	0.83	2/7637 (0.0%)	0.94	4/10315 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	VAL	CA-CB	6.29	1.60	1.53
1	C	58	ALA	CA-CB	5.33	1.61	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	VAL	CB-CA-C	5.53	117.66	111.80
1	B	129	SER	N-CA-C	5.46	116.57	108.60
1	D	99	VAL	CB-CA-C	5.25	118.59	110.82
1	A	128	VAL	N-CA-CB	5.23	117.55	111.90

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	1878	0	1879	39	0
1	B	1882	0	1883	26	0
1	C	1844	0	1848	25	0
1	D	1840	0	1844	36	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
3	C	9	0	0	0	0
3	D	9	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	94	0	0	4	0
6	B	97	0	0	4	0
6	C	110	0	0	2	0
6	D	108	0	0	2	0
All	All	7955	0	7470	115	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 8.

All (115) 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:74[B]:CYS:SG	1:A:83:PHE:CD1	2.22	1.32
1:C:76:LEU:HG	6:C:258:HOH:O	1.30	1.25
1:D:227:LYS:HE3	1:D:228:ALA:O	1.39	1.20
1:C:128:VAL:HG21	1:D:129:SER:O	1.49	1.13
1:A:74[B]:CYS:SG	1:A:83:PHE:CE1	2.43	1.11
1:A:113:VAL:HG13	1:A:125:LEU:HD11	1.33	1.09
1:A:84:THR:HG21	1:B:84:THR:HG21	1.36	1.07
1:A:113:VAL:CG1	1:A:125:LEU:HD11	1.85	1.06
1:B:48:GLY:H	1:C:52:ASN:HD21	1.10	0.97
1:D:227:LYS:CE	1:D:228:ALA:O	2.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:VAL:HG13	1:B:125:LEU:HD11	1.51	0.92
1:C:63:LYS:HE2	6:C:244:HOH:O	1.71	0.89
1:D:72:ILE:HD11	1:D:83:PHE:CE1	2.08	0.89
1:B:113:VAL:CG1	1:B:125:LEU:HD11	2.06	0.85
1:D:129:SER:OG	1:D:130:GLU:HA	1.77	0.84
1:C:84:THR:HG21	1:D:84:THR:HG21	1.61	0.82
1:A:113:VAL:HG13	1:A:125:LEU:CD1	2.11	0.81
1:D:72:ILE:HD11	1:D:83:PHE:CD1	2.16	0.81
1:D:41:THR:HG22	1:D:219:ASN:HB3	1.66	0.75
1:A:128:VAL:HG22	6:A:424:HOH:O	1.92	0.68
1:D:129:SER:CB	1:D:130:GLU:HA	2.20	0.68
1:D:63:LYS:HE2	6:D:243:HOH:O	1.93	0.68
1:B:48:GLY:H	1:C:52:ASN:ND2	1.89	0.67
1:B:41:THR:CG2	1:B:217:LEU:HB2	2.25	0.67
1:C:45:VAL:HG12	1:C:49:VAL:HG13	1.77	0.67
1:C:92[A]:ARG:HG2	1:C:92[A]:ARG:HH11	1.60	0.66
1:A:62:LYS:NZ	1:A:94:HIS:HD2	1.95	0.65
1:D:72:ILE:HD11	1:D:83:PHE:HE1	1.61	0.64
1:B:41:THR:HG22	1:B:217:LEU:HB2	1.80	0.64
1:A:219:ASN:ND2	1:A:222:GLY:H	1.96	0.63
1:D:72:ILE:CD1	1:D:143:VAL:HG21	2.29	0.63
1:C:84:THR:HG21	1:D:84:THR:CG2	2.29	0.62
1:A:21:ASP:OD1	1:A:196:HIS:HE1	1.82	0.62
1:C:84:THR:CG2	1:D:84:THR:HG21	2.29	0.62
1:A:196:HIS:HD2	6:A:287:HOH:O	1.84	0.61
1:B:48:GLY:N	1:C:52:ASN:HD21	1.90	0.61
1:C:45:VAL:HG12	1:C:49:VAL:CG1	2.32	0.60
1:C:76:LEU:HD11	1:C:110:TYR:HD2	1.68	0.59
1:A:74[A]:CYS:SG	1:A:79:SER:OG	2.61	0.58
1:B:113:VAL:HG13	1:B:125:LEU:CD1	2.32	0.58
1:A:219:ASN:C	1:A:219:ASN:HD22	2.11	0.58
1:A:128:VAL:O	6:A:424:HOH:O	2.17	0.56
1:A:80:ARG:HD2	6:A:283:HOH:O	2.05	0.55
1:B:201:TYR:O	1:B:202:SER:HB2	2.07	0.54
1:D:129:SER:H	1:D:130:GLU:HG3	1.72	0.54
1:B:111:VAL:HG22	1:B:129:SER:CB	2.39	0.53
1:A:47:ASN:HD21	1:A:51:LYS:NZ	2.06	0.53
1:D:111:VAL:HG22	1:D:129:SER:HB3	1.90	0.53
1:A:145:ASP:HB2	1:A:203:LEU:HD11	1.91	0.53
1:C:113:VAL:HG13	1:C:125:LEU:HD11	1.90	0.53
1:D:72:ILE:CD1	1:D:83:PHE:HE1	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:HIS:H	1:C:35:HIS:CD2	2.27	0.52
1:D:72:ILE:CG1	1:D:83:PHE:HE1	2.21	0.52
1:D:89:HIS:HD2	6:D:249:HOH:O	1.93	0.51
1:A:62:LYS:HZ2	1:A:94:HIS:HD2	1.57	0.51
1:C:201:TYR:O	1:C:202:SER:HB2	2.10	0.51
1:A:219:ASN:HD22	1:A:222:GLY:H	1.59	0.51
1:D:147:ILE:HG13	1:D:172:CYS:SG	2.50	0.51
1:D:103:LYS:HB2	1:D:104:PRO:CD	2.42	0.50
1:C:45:VAL:CG1	1:C:49:VAL:HG13	2.41	0.50
1:A:73:LEU:C	1:A:73:LEU:HD23	2.37	0.50
1:D:72:ILE:HD13	1:D:143:VAL:HG21	1.94	0.49
1:A:74[B]:CYS:SG	1:A:83:PHE:CG	2.84	0.49
1:D:203:LEU:HD23	1:D:203:LEU:N	2.28	0.48
1:B:140:VAL:HG13	1:B:165:ILE:CG2	2.44	0.48
1:A:135:LEU:HB3	1:A:165:ILE:HG12	1.96	0.47
1:A:35:HIS:H	1:A:35:HIS:CD2	2.31	0.47
1:B:140:VAL:HG13	1:B:165:ILE:HG21	1.95	0.47
1:D:46:PRO:O	1:D:49:VAL:HG12	2.15	0.47
1:C:142:ILE:HD12	1:C:170:ILE:CD1	2.44	0.47
1:B:135:LEU:HB3	1:B:165:ILE:HG12	1.97	0.46
1:D:103:LYS:HB2	1:D:104:PRO:HD2	1.95	0.46
1:A:21:ASP:HA	1:A:194:PRO:HG3	1.97	0.46
1:A:176:LYS:HD3	1:A:195:ASP:HA	1.97	0.46
1:A:74[A]:CYS:HG	1:A:79:SER:HG	1.54	0.46
1:D:147:ILE:HG12	1:D:153:LEU:HD12	1.98	0.46
1:A:89:HIS:HD2	1:A:92:ARG:NH2	2.14	0.46
1:D:35:HIS:H	1:D:35:HIS:CD2	2.33	0.46
1:A:147:ILE:HG12	1:A:153:LEU:HD12	1.98	0.45
1:B:172:CYS:SG	1:B:174:PHE:O	2.74	0.45
1:C:147:ILE:HG12	1:C:153:LEU:HD12	1.99	0.45
1:C:158:GLU:O	1:C:161:LYS:HB2	2.15	0.45
1:A:21:ASP:OD1	1:A:196:HIS:CE1	2.67	0.45
1:A:62:LYS:HZ3	1:A:94:HIS:HD2	1.64	0.45
1:D:72:ILE:CD1	1:D:143:VAL:CG2	2.94	0.45
1:D:140:VAL:HG13	1:D:165:ILE:CG2	2.46	0.45
1:C:128:VAL:CG2	1:D:129:SER:O	2.41	0.44
1:D:72:ILE:HD12	1:D:143:VAL:CG2	2.47	0.44
1:A:198:VAL:HG12	1:A:217:LEU:HD23	2.00	0.44
1:A:201:TYR:O	1:A:202:SER:HB2	2.18	0.44
1:B:132:LEU:O	1:B:135:LEU:HB2	2.18	0.44
1:B:111:VAL:HG13	1:B:129:SER:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLU:OE2	6:B:244:HOH:O	2.21	0.43
1:B:111:VAL:HG22	1:B:129:SER:HB3	2.00	0.43
1:D:70:PHE:O	1:D:106:PHE:HA	2.19	0.43
1:B:35:HIS:CE1	6:B:267:HOH:O	2.71	0.43
1:A:89:HIS:CD2	1:A:92:ARG:HH22	2.38	0.42
1:C:203:LEU:N	1:C:203:LEU:HD12	2.34	0.42
1:B:35:HIS:HE1	6:B:267:HOH:O	2.01	0.42
1:B:1:MET:HA	1:B:2:PRO:HD3	1.73	0.41
1:B:35:HIS:CD2	1:B:35:HIS:H	2.39	0.41
1:D:148:ASP:HB3	4:D:232:PO4:O1	2.20	0.41
1:C:146:ILE:HA	1:C:174:PHE:O	2.20	0.41
1:A:48:GLY:HA3	1:D:48:GLY:C	2.45	0.41
1:D:37:LYS:HE2	1:D:37:LYS:HB2	1.64	0.41
1:A:113:VAL:HG11	1:A:125:LEU:HD11	1.92	0.41
1:D:118:ASN:HD21	1:D:227:LYS:NZ	2.18	0.41
1:B:176:LYS:HD3	1:B:195:ASP:OD1	2.21	0.41
1:C:46:PRO:O	1:C:49:VAL:HG12	2.21	0.41
1:A:130:GLU:HB2	1:B:128:VAL:HG11	2.02	0.41
1:A:83:PHE:CE1	1:A:87:LEU:HD11	2.56	0.40
1:A:47:ASN:HD21	1:A:51:LYS:HZ1	1.69	0.40
1:C:70:PHE:O	1:C:106:PHE:HA	2.22	0.40
1:A:35:HIS:CE1	6:B:249:HOH:O	2.74	0.40
1:B:70:PHE:O	1:B:106:PHE:HA	2.21	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	232/250 (93%)	223 (96%)	9 (4%)	0	100	100
1	B	232/250 (93%)	222 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	227/250 (91%)	217 (96%)	10 (4%)	0	100	100
1	D	227/250 (91%)	217 (96%)	10 (4%)	0	100	100
All	All	918/1000 (92%)	879 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/221 (95%)	200 (96%)	9 (4%)	26	13
1	B	209/221 (95%)	199 (95%)	10 (5%)	23	10
1	C	205/221 (93%)	194 (95%)	11 (5%)	20	7
1	D	205/221 (93%)	188 (92%)	17 (8%)	10	2
All	All	828/884 (94%)	781 (94%)	47 (6%)	19	6

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	26	ASP
1	A	76	LEU
1	A	100	GLU
1	A	113	VAL
1	A	128	VAL
1	A	135	LEU
1	A	141	LEU
1	A	219	ASN
1	B	26	ASP
1	B	75	LEU
1	B	76	LEU
1	B	100	GLU
1	B	126	GLU

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Mol	Chain	Res	Type
1	B	135	LEU
1	B	140	VAL
1	B	162	LYS
1	B	172	CYS
1	B	185	LYS
1	C	57	LEU
1	C	92[A]	ARG
1	C	92[B]	ARG
1	C	103	LYS
1	C	113	VAL
1	C	126	GLU
1	C	128	VAL
1	C	135	LEU
1	C	141	LEU
1	C	154	VAL
1	C	162	LYS
1	D	37	LYS
1	D	41	THR
1	D	57	LEU
1	D	72	ILE
1	D	75	LEU
1	D	76	LEU
1	D	99	VAL
1	D	100	GLU
1	D	103	LYS
1	D	124	THR
1	D	130	GLU
1	D	136	LYS
1	D	140	VAL
1	D	141	LEU
1	D	162	LYS
1	D	203	LEU
1	D	227	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	35	HIS
1	A	47	ASN
1	A	89	HIS
1	A	94	HIS

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Mol	Chain	Res	Type
1	A	196	HIS
1	A	219	ASN
1	B	6	ASN
1	B	35	HIS
1	C	6	ASN
1	C	20	ASN
1	C	35	HIS
1	C	52	ASN
1	C	67	ASN
1	D	12	ASN
1	D	20	ASN
1	D	35	HIS
1	D	89	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
4	PO4	D	232	-	4,4,4	1.24	0	6,6,6	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	POP	A	233	5	6,8,8	0.56	0	12,13,13	1.18	0
3	POP	C	233	5	6,8,8	0.80	0	12,13,13	1.06	2 (16%)
3	POP	B	233	5	6,8,8	0.68	0	12,13,13	1.03	1 (8%)
2	HPA	B	232	-	10,11,11	1.53	2 (20%)	11,15,15	2.49	6 (54%)
2	HPA	A	232	-	10,11,11	1.63	2 (20%)	11,15,15	2.66	7 (63%)
3	POP	D	236	5	6,8,8	0.90	0	12,13,13	1.36	2 (16%)
4	PO4	B	234	-	4,4,4	0.87	0	6,6,6	0.63	0
4	PO4	A	234	-	4,4,4	1.28	0	6,6,6	0.53	0
4	PO4	C	234	-	4,4,4	1.41	0	6,6,6	0.33	0
2	HPA	C	232	-	10,11,11	1.50	1 (10%)	11,15,15	3.11	8 (72%)
2	HPA	D	235	-	10,11,11	1.89	2 (20%)	11,15,15	2.87	8 (72%)

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
3	POP	A	233	5	-	0/6/6/6	-
3	POP	C	233	5	-	0/6/6/6	-
3	POP	B	233	5	-	0/6/6/6	-
2	HPA	B	232	-	-	-	0/2/2/2
2	HPA	A	232	-	-	-	0/2/2/2
3	POP	D	236	5	-	0/6/6/6	-
2	HPA	C	232	-	-	-	0/2/2/2
2	HPA	D	235	-	-	-	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	235	HPA	C2-N3	4.55	1.38	1.30
2	C	232	HPA	C2-N3	4.02	1.37	1.30
2	A	232	HPA	C2-N3	3.66	1.37	1.30
2	B	232	HPA	C2-N3	3.55	1.36	1.30
2	D	235	HPA	C2-N1	2.48	1.40	1.35
2	A	232	HPA	C2-N1	2.34	1.39	1.35
2	B	232	HPA	C2-N1	2.07	1.39	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	235	HPA	N1-C2-N3	-5.54	119.12	125.50
2	C	232	HPA	N1-C2-N3	-4.43	120.39	125.50
2	A	232	HPA	N1-C2-N3	-4.42	120.41	125.50
2	C	232	HPA	C5-C6-N1	4.15	119.36	110.26
2	B	232	HPA	N1-C2-N3	-4.10	120.78	125.50
2	C	232	HPA	C2-N1-C6	-3.84	119.82	125.09
2	A	232	HPA	N7-C8-N9	-3.63	108.77	112.98
2	C	232	HPA	C6-C5-C4	-3.62	119.14	121.61
2	C	232	HPA	N7-C8-N9	-3.59	108.81	112.98
2	D	235	HPA	C5-C6-N1	3.55	118.04	110.26
2	D	235	HPA	N7-C8-N9	-3.48	108.94	112.98
2	B	232	HPA	C5-C6-N1	3.35	117.60	110.26
2	A	232	HPA	C5-C6-N1	3.27	117.44	110.26
2	C	232	HPA	C8-N9-C4	3.25	108.50	102.89
2	D	235	HPA	C8-N9-C4	3.21	108.43	102.89
2	A	232	HPA	C8-N9-C4	3.04	108.13	102.89
2	B	232	HPA	C2-N1-C6	-2.89	121.12	125.09
2	B	232	HPA	C8-N9-C4	2.83	107.77	102.89
2	C	232	HPA	O6-C6-C5	-2.82	120.47	127.26
2	C	232	HPA	C2-N3-C4	2.78	120.19	113.34
2	B	232	HPA	N7-C8-N9	-2.78	109.76	112.98
3	D	236	POP	O2-P1-O	2.67	113.58	104.64
2	A	232	HPA	C2-N1-C6	-2.65	121.45	125.09
2	B	232	HPA	C2-N3-C4	2.62	119.80	113.34
2	D	235	HPA	O6-C6-C5	-2.59	121.01	127.26
2	D	235	HPA	C2-N3-C4	2.58	119.70	113.34
2	A	232	HPA	C2-N3-C4	2.52	119.56	113.34
3	D	236	POP	O6-P2-O	2.47	112.93	104.64
2	D	235	HPA	C6-C5-C4	-2.35	120.01	121.61
2	D	235	HPA	C2-N1-C6	-2.33	121.89	125.09
3	C	233	POP	O3-P1-O	2.08	111.61	104.64
3	C	233	POP	O5-P2-O	2.04	111.47	104.64
3	B	233	POP	O5-P2-O	2.02	111.41	104.64
2	A	232	HPA	C6-C5-C4	-2.01	120.24	121.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	232	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	233/250 (93%)	-1.40	0 100 100	11, 19, 32, 42	1 (0%)
1	B	234/250 (93%)	-1.39	0 100 100	11, 20, 35, 42	0
1	C	228/250 (91%)	-1.41	0 100 100	9, 19, 32, 39	1 (0%)
1	D	228/250 (91%)	-1.41	0 100 100	12, 19, 33, 44	1 (0%)
All	All	923/1000 (92%)	-1.40	0 100 100	9, 19, 33, 44	3 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	HPA	A	232	10/10	0.99	0.03	15,17,18,18	0
2	HPA	B	232	10/10	0.99	0.02	16,18,19,19	0
3	POP	A	233	9/9	0.99	0.04	25,26,27,27	0
3	POP	B	233	9/9	0.99	0.03	28,30,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	235	1/1	0.99	0.04	28,28,28,28	0
5	MG	C	235	1/1	0.99	0.02	20,20,20,20	0
5	MG	C	236	1/1	0.99	0.02	34,34,34,34	0
5	MG	D	234	1/1	0.99	0.02	33,33,33,33	0
4	PO4	A	234	5/5	1.00	0.02	17,18,21,22	0
4	PO4	B	234	5/5	1.00	0.02	17,19,23,24	0
4	PO4	C	234	5/5	1.00	0.02	15,16,19,20	0
4	PO4	D	232	5/5	1.00	0.01	17,17,18,21	0
2	HPA	C	232	10/10	1.00	0.02	11,12,13,13	0
5	MG	B	235	1/1	1.00	0.02	24,24,24,24	0
2	HPA	D	235	10/10	1.00	0.02	11,13,16,16	0
3	POP	C	233	9/9	1.00	0.03	17,18,19,19	0
5	MG	D	233	1/1	1.00	0.04	19,19,19,19	0
3	POP	D	236	9/9	1.00	0.03	16,17,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.