



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:33 AM GMT

PDB ID : 3PDK
Title : crystal structure of phosphoglucosamine mutase from B. anthracis
Authors : Mehra-Chaudhary, R.; Mick, J.; Tanner, J.J.; Henzl, M.; Beamer, L.J.
Deposited on : 2010-10-22
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

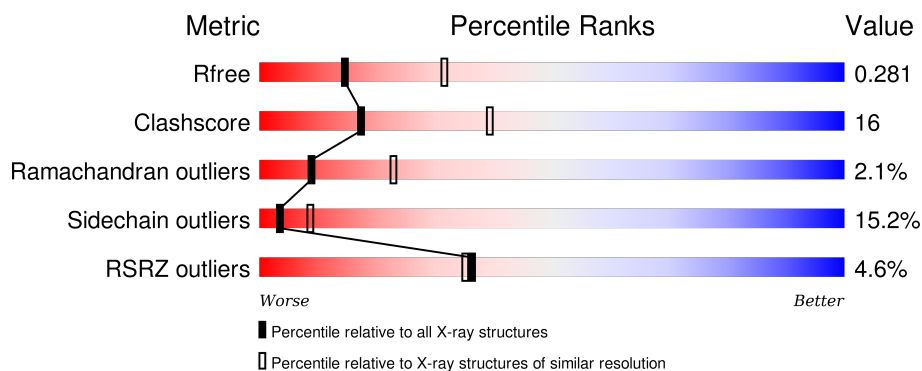
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	469	<div> <div>3%</div> <div>62%</div> <div>26%</div> <div>6%</div> <div>5%</div> </div>
1	B	469	<div> <div>6%</div> <div>63%</div> <div>25%</div> <div>6%</div> <div>5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	450	-	-	-	X
2	PO4	B	449	-	-	X	-
2	PO4	B	451	-	-	X	-
2	PO4	B	453	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6492 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 Phosphoglucosamine mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3220	2017	538	646	19			
1	B	444	Total	C	N	O	S	0	0	0
			3215	2018	538	640	19			

There are 42 discrepancies between the modelled and reference sequences:

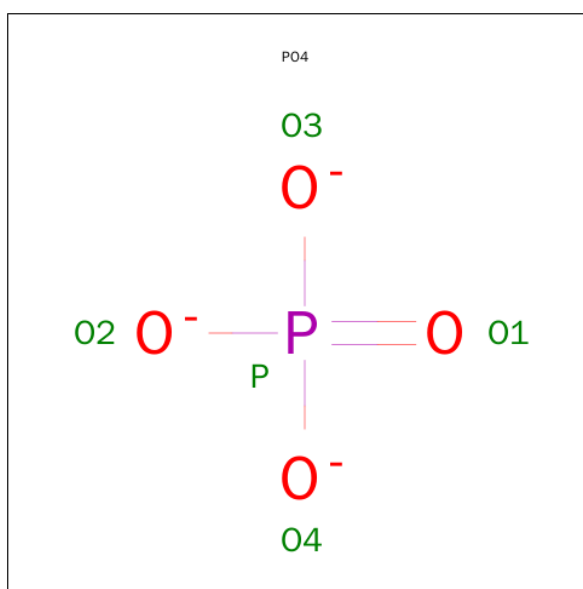
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP Q81VN7
A	-19	SER	-	EXPRESSION TAG	UNP Q81VN7
A	-18	TYR	-	EXPRESSION TAG	UNP Q81VN7
A	-17	TYR	-	EXPRESSION TAG	UNP Q81VN7
A	-16	HIS	-	EXPRESSION TAG	UNP Q81VN7
A	-15	HIS	-	EXPRESSION TAG	UNP Q81VN7
A	-14	HIS	-	EXPRESSION TAG	UNP Q81VN7
A	-13	HIS	-	EXPRESSION TAG	UNP Q81VN7
A	-12	HIS	-	EXPRESSION TAG	UNP Q81VN7
A	-11	HIS	-	EXPRESSION TAG	UNP Q81VN7
A	-10	LEU	-	EXPRESSION TAG	UNP Q81VN7
A	-9	GLU	-	EXPRESSION TAG	UNP Q81VN7
A	-8	SER	-	EXPRESSION TAG	UNP Q81VN7
A	-7	THR	-	EXPRESSION TAG	UNP Q81VN7
A	-6	SER	-	EXPRESSION TAG	UNP Q81VN7
A	-5	LEU	-	EXPRESSION TAG	UNP Q81VN7
A	-4	TYR	-	EXPRESSION TAG	UNP Q81VN7
A	-3	LYS	-	EXPRESSION TAG	UNP Q81VN7
A	-2	LYS	-	EXPRESSION TAG	UNP Q81VN7
A	-1	ALA	-	EXPRESSION TAG	UNP Q81VN7
A	0	GLY	-	EXPRESSION TAG	UNP Q81VN7
B	-20	MET	-	EXPRESSION TAG	UNP Q81VN7
B	-19	SER	-	EXPRESSION TAG	UNP Q81VN7
B	-18	TYR	-	EXPRESSION TAG	UNP Q81VN7
B	-17	TYR	-	EXPRESSION TAG	UNP Q81VN7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	HIS	-	EXPRESSION TAG	UNP Q81VN7
B	-15	HIS	-	EXPRESSION TAG	UNP Q81VN7
B	-14	HIS	-	EXPRESSION TAG	UNP Q81VN7
B	-13	HIS	-	EXPRESSION TAG	UNP Q81VN7
B	-12	HIS	-	EXPRESSION TAG	UNP Q81VN7
B	-11	HIS	-	EXPRESSION TAG	UNP Q81VN7
B	-10	LEU	-	EXPRESSION TAG	UNP Q81VN7
B	-9	GLU	-	EXPRESSION TAG	UNP Q81VN7
B	-8	SER	-	EXPRESSION TAG	UNP Q81VN7
B	-7	THR	-	EXPRESSION TAG	UNP Q81VN7
B	-6	SER	-	EXPRESSION TAG	UNP Q81VN7
B	-5	LEU	-	EXPRESSION TAG	UNP Q81VN7
B	-4	TYR	-	EXPRESSION TAG	UNP Q81VN7
B	-3	LYS	-	EXPRESSION TAG	UNP Q81VN7
B	-2	LYS	-	EXPRESSION TAG	UNP Q81VN7
B	-1	ALA	-	EXPRESSION TAG	UNP Q81VN7
B	0	GLY	-	EXPRESSION TAG	UNP Q81VN7

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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

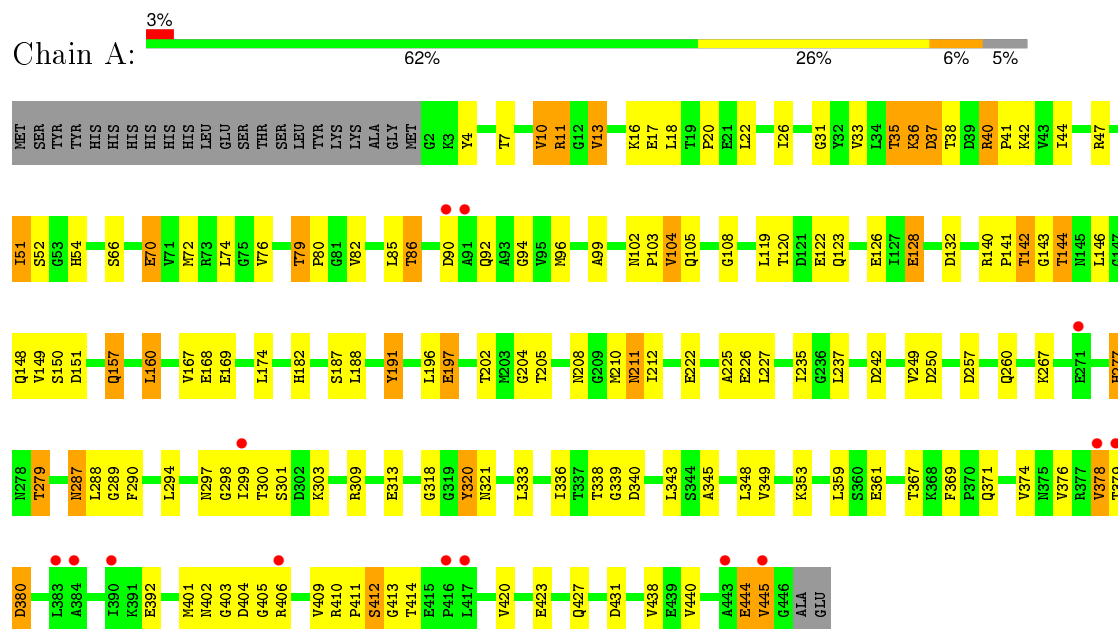
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total	O	0	0
			9	9		
3	B	8	Total	O	0	0
			8	8		

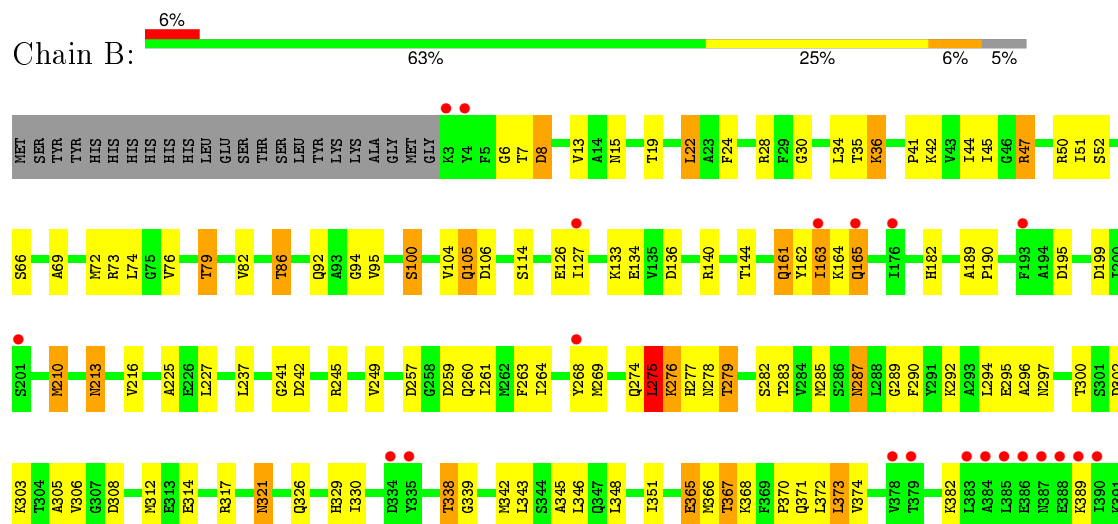
3 Residue-property plots [i](#)

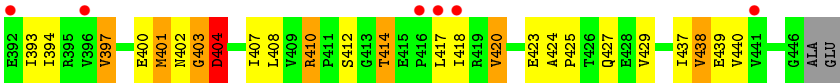
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Phosphoglucosamine mutase



• Molecule 1: Phosphoglucosamine mutase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.06 Å 86.06 Å 266.84 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.03 – 2.70 43.03 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.03-2.70) 98.9 (43.03-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.214 , 0.281 0.217 , 0.281	Depositor DCC
R_{free} test set	1626 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.7	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	1 of 32089 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6492	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.83	1/3267 (0.0%)	0.91	2/4436 (0.0%)
1	B	0.78	1/3262 (0.0%)	0.90	5/4428 (0.1%)
All	All	0.81	2/6529 (0.0%)	0.91	7/8864 (0.1%)

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	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	TYR	CE2-CZ	6.46	1.47	1.38
1	B	295	GLU	CG-CD	5.41	1.60	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	373	LEU	CA-CB-CG	5.91	128.88	115.30
1	B	275	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	34	LEU	CA-CB-CG	5.42	127.78	115.30
1	A	151	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	321	ASN	N-CA-CB	-5.25	101.15	110.60
1	B	47	ARG	NE-CZ-NH2	-5.20	117.70	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	TYR	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	3220	0	3057	101	0
1	B	3215	0	3068	109	0
2	A	15	0	0	0	0
2	B	25	0	0	4	0
3	A	9	0	0	1	0
3	B	8	0	0	1	0
All	All	6492	0	6125	203	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 (203) 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:B:401:MET:O	1:B:404:ASP:HB3	1.43	1.18
1:A:374:VAL:HG21	1:A:438:VAL:HG21	1.25	1.14
1:B:403:GLY:HA3	1:B:404:ASP:HB2	1.38	1.01
1:A:31:GLY:O	1:A:35:THR:HB	1.65	0.97
1:B:403:GLY:CA	1:B:404:ASP:HB2	1.96	0.96
1:A:82:VAL:O	1:A:86:THR:HG23	1.69	0.93
1:A:287:ASN:HD21	1:A:369:PHE:H	1.19	0.86
1:B:42:LYS:HD3	1:B:72:MET:CE	2.07	0.84
1:A:374:VAL:CG2	1:A:438:VAL:HG21	2.07	0.84
1:B:42:LYS:H	1:B:92:GLN:HE22	1.23	0.83
1:B:437:ILE:O	1:B:440:VAL:HB	1.78	0.82
1:A:44:ILE:HD11	1:A:86:THR:HG22	1.62	0.82
1:B:42:LYS:H	1:B:92:GLN:NE2	1.79	0.80
1:A:211:ASN:H	1:A:211:ASN:HD22	1.30	0.78
1:A:374:VAL:HG21	1:A:438:VAL:CG2	2.11	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:HA	1:A:92:GLN:NE2	2.01	0.74
1:A:379:THR:O	1:A:380:ASP:HB3	1.88	0.73
1:B:82:VAL:O	1:B:86:THR:HG22	1.88	0.73
1:A:277:HIS:O	1:A:279:THR:HG23	1.89	0.72
1:B:393:ILE:HD11	1:B:440:VAL:HG11	1.69	0.71
1:A:182:HIS:CE1	1:A:204:GLY:HA2	2.25	0.71
1:B:42:LYS:HD3	1:B:72:MET:HE3	1.71	0.71
1:B:397:VAL:O	1:B:400:GLU:HB2	1.91	0.71
1:A:36:LYS:HB3	1:A:37:ASP:OD1	1.92	0.69
1:A:235:ILE:HD12	1:A:359:LEU:HD22	1.74	0.69
1:B:296:ALA:O	1:B:297:ASN:HB2	1.92	0.69
1:B:42:LYS:N	1:B:92:GLN:HE22	1.91	0.68
1:B:287:ASN:HB3	1:B:371:GLN:OE1	1.94	0.68
1:B:213:ASN:HD21	1:B:241:GLY:H	1.40	0.67
1:B:269:MET:HB3	1:B:275:LEU:HB2	1.77	0.67
1:B:275:LEU:HD13	1:B:278:ASN:HA	1.75	0.67
1:A:257:ASP:H	1:A:260:GLN:HE21	1.43	0.66
1:B:412:SER:O	2:B:449:PO4:O4	2.14	0.65
1:A:297:ASN:O	1:A:299:ILE:N	2.30	0.65
1:A:287:ASN:ND2	1:A:289:GLY:H	1.95	0.65
1:B:279:THR:HG22	1:B:300:THR:HB	1.79	0.65
1:A:277:HIS:O	1:A:279:THR:CG2	2.45	0.64
1:B:285:MET:HE1	1:B:408:LEU:HD21	1.78	0.64
1:A:257:ASP:H	1:A:260:GLN:NE2	1.96	0.64
1:B:164:LYS:HE3	1:B:195:ASP:OD2	1.98	0.63
1:A:51:ILE:CG2	1:A:52:SER:N	2.61	0.63
1:B:285:MET:CE	1:B:408:LEU:CD2	2.76	0.63
1:A:20:PRO:HB2	1:B:24:PHE:CE1	2.33	0.63
1:B:86:THR:HG21	1:B:94:GLY:HA3	1.80	0.62
1:A:294:LEU:O	1:A:299:ILE:HB	1.99	0.61
1:A:41:PRO:HA	1:A:92:GLN:HE22	1.63	0.60
1:B:41:PRO:HG2	1:B:69:ALA:HA	1.84	0.60
1:B:410:ARG:NH2	2:B:449:PO4:O1	2.34	0.60
1:A:318:GLY:HA3	1:A:320:TYR:CE2	2.37	0.60
1:A:4:TYR:N	1:A:128:GLU:OE2	2.33	0.60
1:A:120:THR:OG1	1:A:123:GLN:HG3	2.02	0.60
1:A:86:THR:HG21	1:A:94:GLY:HA3	1.83	0.60
1:B:140:ARG:HD2	3:B:455:HOH:O	2.00	0.59
1:A:402:ASN:CB	1:A:403:GLY:HA2	2.31	0.59
1:A:144:THR:HA	1:B:210:MET:HE1	1.85	0.59
1:B:285:MET:HE1	1:B:408:LEU:CD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ILE:HG23	1:A:52:SER:N	2.18	0.58
1:B:163:ILE:HG23	1:B:346:LEU:HD11	1.85	0.58
1:B:277:HIS:O	1:B:279:THR:HG23	2.04	0.57
1:A:80:PRO:HG3	1:A:339:GLY:O	2.04	0.57
1:B:314:GLU:HA	1:B:314:GLU:OE1	2.04	0.57
1:A:211:ASN:N	1:A:211:ASN:HD22	2.01	0.57
1:A:82:VAL:O	1:A:86:THR:CG2	2.50	0.57
1:B:268:TYR:CG	1:B:351:ILE:HD12	2.40	0.56
1:A:287:ASN:ND2	1:A:369:PHE:H	1.99	0.56
1:B:329:HIS:CE1	2:B:451:PO4:O3	2.59	0.56
1:B:424:ALA:HB1	1:B:425:PRO:CD	2.36	0.56
1:A:90:ASP:HA	3:A:456:HOH:O	2.04	0.56
1:B:312:MET:HA	1:B:312:MET:HE3	1.87	0.56
1:A:374:VAL:CG2	1:A:438:VAL:CG2	2.78	0.56
1:B:163:ILE:HG13	1:B:343:LEU:HD13	1.88	0.55
1:A:378:VAL:HA	1:A:445:VAL:HG13	1.89	0.55
1:B:289:GLY:HA3	1:B:367:THR:O	2.06	0.55
1:B:403:GLY:HA3	1:B:404:ASP:CB	2.27	0.55
1:B:82:VAL:O	1:B:86:THR:CG2	2.53	0.55
1:B:279:THR:HA	1:B:300:THR:O	2.07	0.55
1:B:269:MET:CB	1:B:275:LEU:HB2	2.37	0.55
1:A:376:VAL:HG21	1:A:438:VAL:HG22	1.89	0.54
1:B:161:GLN:HA	1:B:161:GLN:NE2	2.22	0.54
1:A:79:THR:HG22	1:A:242:ASP:HB2	1.90	0.54
1:A:401:MET:HE1	1:A:405:GLY:HA3	1.88	0.54
1:A:208:ASN:H	1:A:211:ASN:HD21	1.56	0.54
1:A:13:VAL:HG22	1:A:16:LYS:HB3	1.89	0.54
1:A:225:ALA:HA	1:A:249:VAL:HG11	1.90	0.54
1:A:287:ASN:ND2	1:A:289:GLY:N	2.57	0.53
1:B:393:ILE:CD1	1:B:440:VAL:HG11	2.37	0.52
1:B:329:HIS:NE2	2:B:451:PO4:O3	2.43	0.52
1:B:276:LYS:H	1:B:321:ASN:ND2	2.08	0.52
1:B:28:ARG:NH1	1:B:66:SER:OG	2.42	0.52
1:A:202:THR:HB	1:A:205:THR:HG21	1.91	0.51
1:B:42:LYS:HD3	1:B:72:MET:HE1	1.89	0.51
1:B:389:LYS:O	1:B:393:ILE:HD11	2.11	0.51
1:A:47:ARG:O	1:A:76:VAL:HA	2.11	0.51
1:B:28:ARG:HH22	1:B:140:ARG:HG2	1.76	0.51
1:A:79:THR:HB	1:A:96:MET:HG2	1.92	0.50
1:B:314:GLU:OE1	1:B:317:ARG:NH1	2.44	0.50
1:A:40:ARG:N	1:A:41:PRO:HD3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:VAL:HG13	1:A:17:GLU:OE1	2.11	0.50
1:B:105:GLN:OE1	1:B:105:GLN:N	2.40	0.50
1:B:285:MET:CE	1:B:306:VAL:HG21	2.41	0.50
1:A:44:ILE:HG22	1:A:72:MET:HB2	1.94	0.50
1:B:285:MET:CE	1:B:408:LEU:HD23	2.41	0.50
1:A:250:ASP:C	1:A:250:ASP:OD2	2.51	0.49
1:B:285:MET:HE1	1:B:306:VAL:HG21	1.92	0.49
1:A:287:ASN:HD22	1:A:289:GLY:N	2.10	0.49
1:B:275:LEU:CD1	1:B:278:ASN:HA	2.42	0.49
1:A:148:GLN:HG2	1:B:51:ILE:HD11	1.95	0.49
1:A:340:ASP:HB3	1:A:343:LEU:HB3	1.94	0.49
1:A:427:GLN:HG3	1:A:431:ASP:OD2	2.12	0.49
1:B:403:GLY:N	1:B:404:ASP:HB2	2.28	0.49
1:A:79:THR:N	1:A:80:PRO:HD2	2.28	0.49
1:B:237:LEU:HD13	1:B:345:ALA:HB1	1.94	0.49
1:A:11:ARG:NH1	1:A:99:ALA:HA	2.28	0.49
1:B:260:GLN:O	1:B:264:ILE:HG13	2.12	0.49
1:B:162:TYR:O	1:B:165:GLN:NE2	2.31	0.49
1:B:285:MET:CE	1:B:408:LEU:HD21	2.42	0.48
1:B:100:SER:HA	1:B:242:ASP:OD2	2.13	0.48
1:A:104:VAL:HG13	1:A:212:ILE:HG22	1.96	0.48
1:B:41:PRO:HA	1:B:92:GLN:HE22	1.77	0.48
1:A:37:ASP:OD1	1:A:37:ASP:N	2.44	0.48
1:B:342:MET:O	1:B:345:ALA:HB3	2.14	0.48
1:B:257:ASP:H	1:B:260:GLN:NE2	2.12	0.48
1:A:54:HIS:CD2	1:A:54:HIS:H	2.32	0.48
1:A:440:VAL:O	1:A:444:GLU:HB2	2.14	0.48
1:A:379:THR:O	1:A:380:ASP:CB	2.59	0.47
1:A:402:ASN:CB	1:A:403:GLY:CA	2.92	0.47
1:B:47:ARG:O	1:B:76:VAL:HA	2.14	0.47
1:A:196:LEU:O	1:A:197:GLU:HB2	2.14	0.47
1:B:374:VAL:O	1:B:420:VAL:HG23	2.14	0.47
1:B:189:ALA:N	1:B:190:PRO:CD	2.78	0.47
1:A:403:GLY:HA3	1:A:404:ASP:HB3	1.96	0.46
1:B:296:ALA:O	1:B:297:ASN:CB	2.61	0.46
1:B:35:THR:O	1:B:36:LYS:C	2.54	0.46
1:B:213:ASN:HD21	1:B:241:GLY:N	2.10	0.46
1:A:42:LYS:HG3	1:A:70:GLU:HG2	1.98	0.46
1:B:438:VAL:O	1:B:439:GLU:C	2.54	0.46
1:A:144:THR:HA	1:B:210:MET:CE	2.46	0.46
1:A:345:ALA:O	1:A:349:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:HE2	1:B:365:GLU:HB3	1.81	0.46
1:A:79:THR:CG2	1:A:242:ASP:HB2	2.46	0.45
1:B:283:THR:C	1:B:285:MET:H	2.19	0.45
1:A:210:MET:HB3	1:B:144:THR:HG22	1.98	0.45
1:B:41:PRO:HA	1:B:92:GLN:NE2	2.30	0.45
1:A:309:ARG:O	1:A:313:GLU:HG2	2.16	0.45
1:A:66:SER:O	1:A:141:PRO:HD2	2.16	0.45
1:A:208:ASN:H	1:A:211:ASN:ND2	2.14	0.44
1:A:250:ASP:HA	1:A:359:LEU:HD23	2.00	0.44
1:B:225:ALA:HA	1:B:249:VAL:HG11	2.00	0.44
1:B:370:PRO:HA	1:B:427:GLN:HE22	1.82	0.44
1:A:376:VAL:CG2	1:A:438:VAL:HG22	2.47	0.44
1:A:157:GLN:HB2	1:A:157:GLN:HE21	1.57	0.44
1:B:44:ILE:HG22	1:B:72:MET:HB2	1.98	0.44
1:A:412:SER:HB2	1:A:413:GLY:H	1.66	0.44
1:A:33:VAL:HG22	1:A:126:GLU:HG2	1.98	0.44
1:B:314:GLU:CD	1:B:317:ARG:HH12	2.21	0.44
1:A:54:HIS:CD2	1:A:54:HIS:N	2.86	0.44
1:A:140:ARG:HD2	1:B:15:ASN:O	2.18	0.44
1:B:261:ILE:HG22	1:B:330:ILE:HD13	2.00	0.44
1:B:45:ILE:HG23	1:B:45:ILE:O	2.18	0.43
1:A:10:VAL:HG11	1:A:26:ILE:HD13	2.00	0.43
1:A:92:GLN:N	1:A:92:GLN:OE1	2.52	0.43
1:B:368:LYS:HE2	1:B:368:LYS:HB3	1.87	0.43
1:A:102:ASN:HB3	1:A:103:PRO:HD2	2.00	0.43
1:B:182:HIS:HD2	1:B:216:VAL:HG21	1.84	0.42
1:A:287:ASN:O	1:A:290:PHE:HB3	2.19	0.42
1:B:268:TYR:CD2	1:B:351:ILE:CD1	3.02	0.42
1:A:237:LEU:HD13	1:A:345:ALA:HB1	2.02	0.42
1:B:8:ASP:HB3	1:B:414:THR:HG21	2.00	0.42
1:B:287:ASN:O	1:B:290:PHE:HB3	2.20	0.42
1:B:282:SER:O	1:B:303:LYS:HA	2.20	0.42
1:B:394:ILE:O	1:B:397:VAL:HG23	2.20	0.42
1:B:285:MET:HB2	1:B:285:MET:HE3	1.75	0.41
1:B:182:HIS:CD2	1:B:216:VAL:HG21	2.55	0.41
1:B:79:THR:HG22	1:B:242:ASP:HB2	2.02	0.41
1:A:10:VAL:O	1:A:108:GLY:HA2	2.20	0.41
1:B:19:THR:OG1	1:B:22:LEU:HB2	2.20	0.41
1:A:290:PHE:O	1:A:294:LEU:HB2	2.19	0.41
1:B:45:ILE:HG13	1:B:95:VAL:HB	2.02	0.41
1:A:142:THR:HG23	1:A:143:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:NH1	1:B:106:ASP:O	2.53	0.41
1:A:149:VAL:HG22	1:A:150:SER:N	2.35	0.41
1:B:268:TYR:CD2	1:B:351:ILE:HD12	2.55	0.41
1:B:424:ALA:HB1	1:B:425:PRO:HD2	2.01	0.41
1:A:409:VAL:HG22	1:A:420:VAL:HA	2.02	0.41
1:B:302:ASP:OD1	1:B:314:GLU:OE2	2.39	0.41
1:B:259:ASP:CG	1:B:326:GLN:HG2	2.41	0.41
1:A:40:ARG:H	1:A:41:PRO:HD3	1.86	0.41
1:A:33:VAL:CG2	1:A:126:GLU:HG2	2.50	0.41
1:B:42:LYS:CD	1:B:72:MET:CE	2.91	0.41
1:A:401:MET:HB3	1:A:401:MET:HE2	1.82	0.41
1:A:406:ARG:HG2	1:A:423:GLU:HB2	2.02	0.41
1:A:336:ILE:HG22	1:A:338:THR:O	2.20	0.41
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.65	0.41
1:B:30:GLY:HA2	1:B:127:ILE:HG12	2.03	0.41
1:A:146:LEU:CD2	1:B:52:SER:HA	2.51	0.41
1:A:294:LEU:O	1:A:297:ASN:O	2.39	0.40
1:B:402:ASN:O	1:B:403:GLY:C	2.59	0.40
1:A:44:ILE:CD1	1:A:86:THR:HG22	2.43	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.83	0.40
1:B:126:GLU:HG2	1:B:126:GLU:O	2.21	0.40
1:A:157:GLN:HA	1:A:160:LEU:HB2	2.02	0.40
1:B:338:THR:OG1	1:B:339:GLY:N	2.54	0.40
1:B:257:ASP:H	1:B:260:GLN:HE21	1.68	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	443/469 (94%)	407 (92%)	27 (6%)	9 (2%)	9 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	442/469 (94%)	388 (88%)	44 (10%)	10 (2%)	8	20
All	All	885/938 (94%)	795 (90%)	71 (8%)	19 (2%)	9	23

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	298	GLY
1	B	36	LYS
1	B	213	ASN
1	B	382	LYS
1	B	403	GLY
1	B	404	ASP
1	A	277	HIS
1	A	380	ASP
1	B	6	GLY
1	B	8	ASP
1	B	134	GLU
1	A	168	GLU
1	A	414	THR
1	B	438	VAL
1	A	378	VAL
1	B	305	ALA
1	A	40	ARG
1	A	411	PRO

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	323/383 (84%)	271 (84%)	52 (16%)	3	7
1	B	322/383 (84%)	276 (86%)	46 (14%)	4	10
All	All	645/766 (84%)	547 (85%)	98 (15%)	3	9

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	10	VAL
1	A	11	ARG
1	A	13	VAL
1	A	22	LEU
1	A	35	THR
1	A	37	ASP
1	A	38	THR
1	A	51	ILE
1	A	70	GLU
1	A	74	LEU
1	A	79	THR
1	A	86	THR
1	A	104	VAL
1	A	105	GLN
1	A	119	LEU
1	A	122	GLU
1	A	128	GLU
1	A	132	ASP
1	A	142	THR
1	A	144	THR
1	A	157	GLN
1	A	160	LEU
1	A	167	VAL
1	A	169	GLU
1	A	174	LEU
1	A	187	SER
1	A	188	LEU
1	A	191	TYR
1	A	197	GLU
1	A	211	ASN
1	A	222	GLU
1	A	226	GLU
1	A	227	LEU
1	A	267	LYS
1	A	279	THR
1	A	287	ASN
1	A	288	LEU
1	A	300	THR
1	A	301	SER
1	A	303	LYS
1	A	333	LEU
1	A	348	LEU

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Mol	Chain	Res	Type
1	A	353	LYS
1	A	361	GLU
1	A	367	THR
1	A	371	GLN
1	A	392	GLU
1	A	410	ARG
1	A	412	SER
1	A	444	GLU
1	A	445	VAL
1	B	7	THR
1	B	13	VAL
1	B	22	LEU
1	B	74	LEU
1	B	79	THR
1	B	86	THR
1	B	100	SER
1	B	104	VAL
1	B	105	GLN
1	B	114	SER
1	B	133	LYS
1	B	136	ASP
1	B	161	GLN
1	B	163	ILE
1	B	165	GLN
1	B	199	ASP
1	B	210	MET
1	B	227	LEU
1	B	245	ARG
1	B	274	GLN
1	B	275	LEU
1	B	276	LYS
1	B	279	THR
1	B	287	ASN
1	B	292	LYS
1	B	294	LEU
1	B	308	ASP
1	B	321	ASN
1	B	338	THR
1	B	348	LEU
1	B	365	GLU
1	B	366	MET
1	B	367	THR

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Mol	Chain	Res	Type
1	B	372	LEU
1	B	373	LEU
1	B	397	VAL
1	B	401	MET
1	B	404	ASP
1	B	407	ILE
1	B	410	ARG
1	B	414	THR
1	B	417	LEU
1	B	418	ILE
1	B	420	VAL
1	B	423	GLU
1	B	429	VAL

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

Mol	Chain	Res	Type
1	A	54	HIS
1	A	92	GLN
1	A	157	GLN
1	A	211	ASN
1	A	260	GLN
1	A	274	GLN
1	A	287	ASN
1	A	297	ASN
1	B	54	HIS
1	B	92	GLN
1	B	161	GLN
1	B	213	ASN
1	B	260	GLN
1	B	321	ASN
1	B	427	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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	A	449	-	4,4,4	0.28	0	6,6,6	0.30	0
2	PO4	A	450	-	4,4,4	0.27	0	6,6,6	0.27	0
2	PO4	A	451	-	4,4,4	0.32	0	6,6,6	0.27	0
2	PO4	B	449	-	4,4,4	0.28	0	6,6,6	0.30	0
2	PO4	B	450	-	4,4,4	0.28	0	6,6,6	0.25	0
2	PO4	B	451	-	4,4,4	0.23	0	6,6,6	0.31	0
2	PO4	B	452	-	4,4,4	0.34	0	6,6,6	0.27	0
2	PO4	B	453	-	4,4,4	0.36	0	6,6,6	0.26	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	PO4	A	449	-	-	0/0/0/0	0/0/0/0
2	PO4	A	450	-	-	0/0/0/0	0/0/0/0
2	PO4	A	451	-	-	0/0/0/0	0/0/0/0
2	PO4	B	449	-	-	0/0/0/0	0/0/0/0
2	PO4	B	450	-	-	0/0/0/0	0/0/0/0
2	PO4	B	451	-	-	0/0/0/0	0/0/0/0
2	PO4	B	452	-	-	0/0/0/0	0/0/0/0
2	PO4	B	453	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	449	PO4	2	0
2	B	451	PO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	445/469 (94%)	0.23	14 (3%) 52 52	57, 83, 127, 178	0
1	B	444/469 (94%)	0.34	27 (6%) 25 23	67, 86, 160, 225	0
All	All	889/938 (94%)	0.28	41 (4%) 36 35	57, 84, 144, 225	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	384	ALA	8.0
1	B	379	THR	6.3
1	A	390	ILE	5.2
1	B	385	LEU	5.1
1	B	390	ILE	5.0
1	A	383	LEU	4.8
1	B	383	LEU	4.4
1	A	379	THR	4.4
1	B	335	TYR	4.2
1	B	387	ASN	4.0
1	B	386	GLU	3.9
1	A	378	VAL	3.9
1	B	388	GLU	3.9
1	A	445	VAL	3.5
1	A	443	ALA	3.4
1	B	441	VAL	3.4
1	B	417	LEU	3.2
1	A	384	ALA	3.0
1	B	268	TYR	3.0
1	B	4	TYR	2.9
1	B	389	LYS	2.9
1	A	406	ARG	2.8
1	B	396	VAL	2.8
1	A	417	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	201	SER	2.7
1	B	416	PRO	2.7
1	A	271	GLU	2.6
1	B	193	PHE	2.5
1	B	378	VAL	2.5
1	B	127	ILE	2.5
1	A	91	ALA	2.4
1	B	392	GLU	2.4
1	A	416	PRO	2.3
1	A	90	ASP	2.3
1	A	299	ILE	2.2
1	B	176	ILE	2.2
1	B	165	GLN	2.2
1	B	418	ILE	2.1
1	B	163	ILE	2.1
1	B	3	LYS	2.1
1	B	334	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	A	450	5/5	0.86	0.45	15.91	140,141,141,141	0
2	PO4	B	453	5/5	0.63	0.41	2.06	157,158,158,158	0
2	PO4	B	451	5/5	0.94	0.24	1.66	117,118,119,120	0
2	PO4	A	449	5/5	0.88	0.18	-0.29	129,129,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	PO4	B	449	5/5	0.94	0.14	-0.66	93,94,95,95	0
2	PO4	B	450	5/5	0.93	0.10	-5.47	120,123,124,125	0
2	PO4	A	451	5/5	0.87	0.14	-	139,140,140,141	0
2	PO4	B	452	5/5	0.89	0.20	-	127,128,128,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.