



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:30 PM UTC

PDB ID : 3LG2 / pdb_00003lg2
Title : A Ykr043C/ fructose-1,6-bisphosphate product complex following ligand soaking
Authors : Singer, A.; Xu, X.; Cui, H.; Dong, A.; Edwards, A.M.; Joachimiak, A.; Yakunin, A.F.; Savchenko, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2010-01-19
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

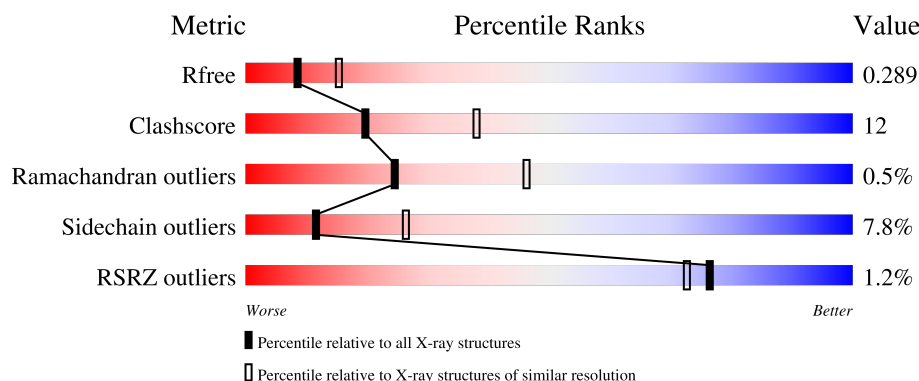
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	292	 66% 25% • 8%
1	B	292	 66% 23% • 8%
1	C	292	 67% 24% • 8%
1	D	292	 68% 21% • 8%

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	B	300	-	-	X	-
2	PO4	B	302	-	-	X	-
2	PO4	C	272	-	-	X	-
2	PO4	C	302	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8732 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 Uncharacterized protein YKR043C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	Se	0	0	0
			2172	1362	391	412	4	3			
1	B	269	Total	C	N	O	S	Se	0	0	0
			2172	1362	391	412	4	3			
1	C	269	Total	C	N	O	S	Se	0	0	0
			2172	1362	391	412	4	3			
1	D	269	Total	C	N	O	S	Se	0	0	0
			2172	1362	391	412	4	3			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MSE	-	expression tag	UNP P36136
A	-19	GLY	-	expression tag	UNP P36136
A	-18	SER	-	expression tag	UNP P36136
A	-17	SER	-	expression tag	UNP P36136
A	-16	HIS	-	expression tag	UNP P36136
A	-15	HIS	-	expression tag	UNP P36136
A	-14	HIS	-	expression tag	UNP P36136
A	-13	HIS	-	expression tag	UNP P36136
A	-12	HIS	-	expression tag	UNP P36136
A	-11	HIS	-	expression tag	UNP P36136
A	-10	SER	-	expression tag	UNP P36136
A	-9	SER	-	expression tag	UNP P36136
A	-8	GLY	-	expression tag	UNP P36136
A	-7	ARG	-	expression tag	UNP P36136
A	-6	GLU	-	expression tag	UNP P36136
A	-5	ASN	-	expression tag	UNP P36136
A	-4	LEU	-	expression tag	UNP P36136
A	-3	TYR	-	expression tag	UNP P36136
A	-2	PHE	-	expression tag	UNP P36136
A	-1	GLN	-	expression tag	UNP P36136
A	0	GLY	-	expression tag	UNP P36136

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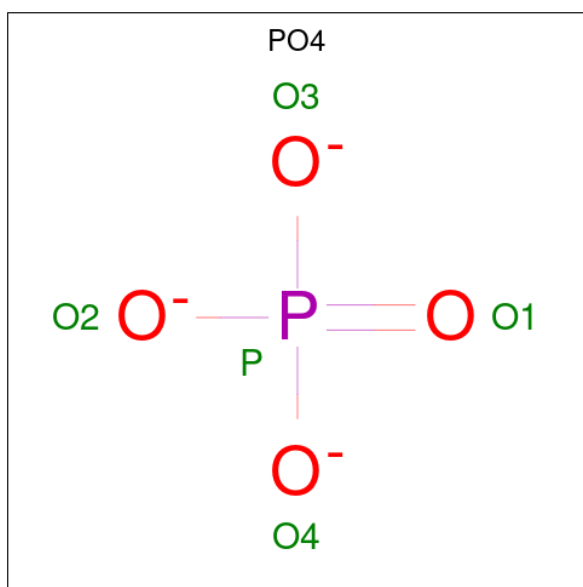
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MSE	-	expression tag	UNP P36136
B	-19	GLY	-	expression tag	UNP P36136
B	-18	SER	-	expression tag	UNP P36136
B	-17	SER	-	expression tag	UNP P36136
B	-16	HIS	-	expression tag	UNP P36136
B	-15	HIS	-	expression tag	UNP P36136
B	-14	HIS	-	expression tag	UNP P36136
B	-13	HIS	-	expression tag	UNP P36136
B	-12	HIS	-	expression tag	UNP P36136
B	-11	HIS	-	expression tag	UNP P36136
B	-10	SER	-	expression tag	UNP P36136
B	-9	SER	-	expression tag	UNP P36136
B	-8	GLY	-	expression tag	UNP P36136
B	-7	ARG	-	expression tag	UNP P36136
B	-6	GLU	-	expression tag	UNP P36136
B	-5	ASN	-	expression tag	UNP P36136
B	-4	LEU	-	expression tag	UNP P36136
B	-3	TYR	-	expression tag	UNP P36136
B	-2	PHE	-	expression tag	UNP P36136
B	-1	GLN	-	expression tag	UNP P36136
B	0	GLY	-	expression tag	UNP P36136
C	-20	MSE	-	expression tag	UNP P36136
C	-19	GLY	-	expression tag	UNP P36136
C	-18	SER	-	expression tag	UNP P36136
C	-17	SER	-	expression tag	UNP P36136
C	-16	HIS	-	expression tag	UNP P36136
C	-15	HIS	-	expression tag	UNP P36136
C	-14	HIS	-	expression tag	UNP P36136
C	-13	HIS	-	expression tag	UNP P36136
C	-12	HIS	-	expression tag	UNP P36136
C	-11	HIS	-	expression tag	UNP P36136
C	-10	SER	-	expression tag	UNP P36136
C	-9	SER	-	expression tag	UNP P36136
C	-8	GLY	-	expression tag	UNP P36136
C	-7	ARG	-	expression tag	UNP P36136
C	-6	GLU	-	expression tag	UNP P36136
C	-5	ASN	-	expression tag	UNP P36136
C	-4	LEU	-	expression tag	UNP P36136
C	-3	TYR	-	expression tag	UNP P36136
C	-2	PHE	-	expression tag	UNP P36136
C	-1	GLN	-	expression tag	UNP P36136
C	0	GLY	-	expression tag	UNP P36136

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MSE	-	expression tag	UNP P36136
D	-19	GLY	-	expression tag	UNP P36136
D	-18	SER	-	expression tag	UNP P36136
D	-17	SER	-	expression tag	UNP P36136
D	-16	HIS	-	expression tag	UNP P36136
D	-15	HIS	-	expression tag	UNP P36136
D	-14	HIS	-	expression tag	UNP P36136
D	-13	HIS	-	expression tag	UNP P36136
D	-12	HIS	-	expression tag	UNP P36136
D	-11	HIS	-	expression tag	UNP P36136
D	-10	SER	-	expression tag	UNP P36136
D	-9	SER	-	expression tag	UNP P36136
D	-8	GLY	-	expression tag	UNP P36136
D	-7	ARG	-	expression tag	UNP P36136
D	-6	GLU	-	expression tag	UNP P36136
D	-5	ASN	-	expression tag	UNP P36136
D	-4	LEU	-	expression tag	UNP P36136
D	-3	TYR	-	expression tag	UNP P36136
D	-2	PHE	-	expression tag	UNP P36136
D	-1	GLN	-	expression tag	UNP P36136
D	0	GLY	-	expression tag	UNP P36136

- 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		

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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	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

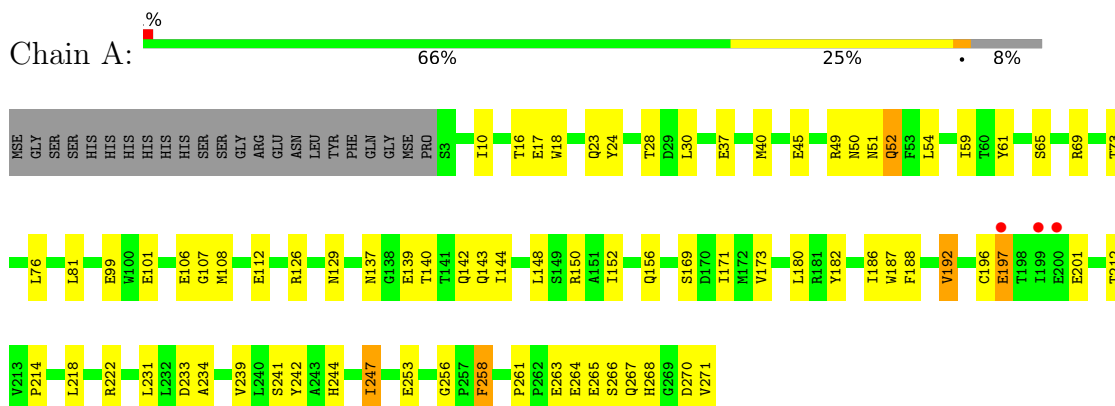
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	2	Total	O	0	0
			2	2		
3	C	1	Total	O	0	0
			1	1		

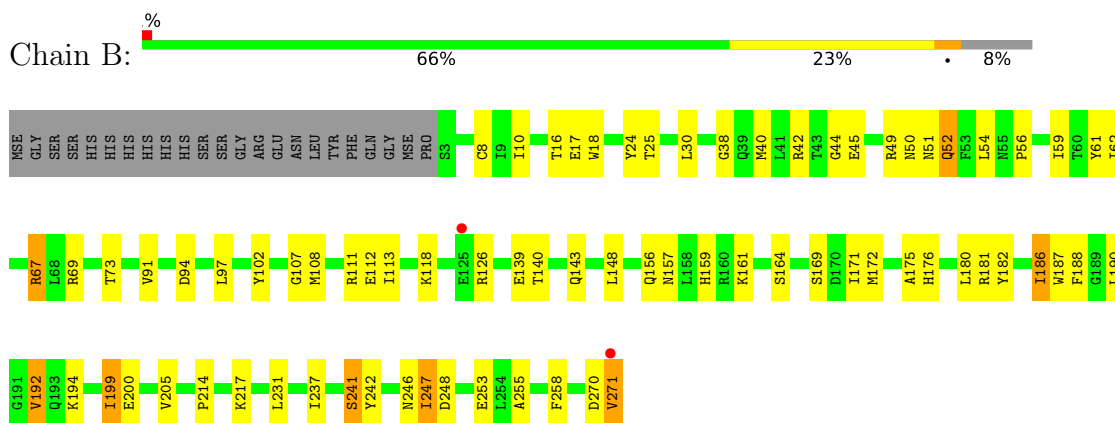
3 Residue-property plots [i](#)

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.

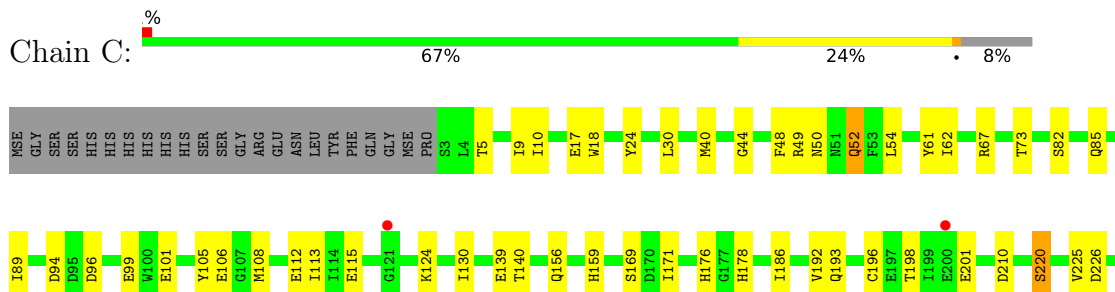
• Molecule 1: Uncharacterized protein YKR043C



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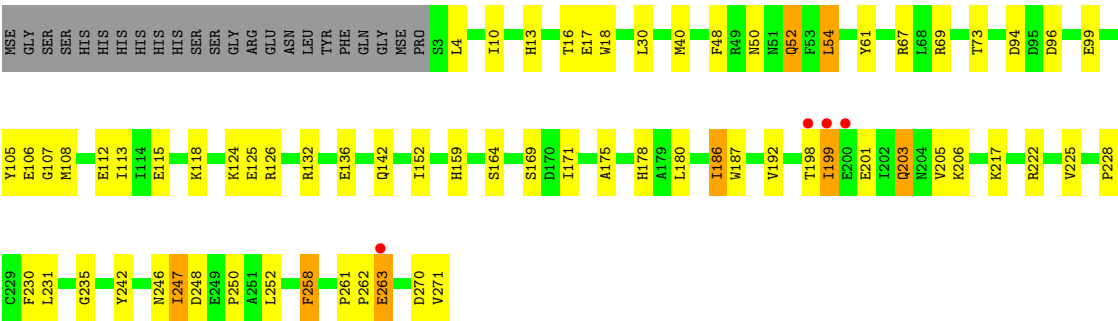


• Molecule 1: Uncharacterized protein YKR043C





● Molecule 1: Uncharacterized protein YKR043C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.30Å 83.39Å 104.69Å 90.00° 104.19° 90.00°	Depositor
Resolution (Å)	43.35 – 2.60 43.35 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.2 (43.35-2.60) 91.1 (43.35-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.220 , 0.270 0.242 , 0.289	Depositor DCC
R_{free} test set	2008 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8732	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1303e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.86	0/2218	1.01	4/2999 (0.1%)
1	B	0.86	0/2218	1.02	3/2999 (0.1%)
1	C	0.99	0/2218	1.06	5/2999 (0.2%)
1	D	1.01	0/2218	1.08	3/2999 (0.1%)
All	All	0.93	0/8872	1.04	15/11996 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	225	VAL	N-CA-C	-6.24	107.21	113.20
1	C	258	PHE	N-CA-C	6.18	118.69	108.99
1	C	169	SER	N-CA-C	6.09	117.40	107.23
1	B	44	GLY	N-CA-C	-6.08	105.45	112.50
1	A	169	SER	N-CA-C	5.97	117.19	107.23
1	D	192	VAL	N-CA-C	5.96	117.06	108.48
1	A	192	VAL	N-CA-C	5.90	116.98	108.48
1	B	192	VAL	N-CA-C	5.71	116.70	108.48
1	D	169	SER	N-CA-C	5.63	116.64	107.23
1	C	44	GLY	N-CA-C	-5.51	106.12	112.73
1	C	226	ASP	N-CA-C	5.41	115.69	108.38
1	B	169	SER	N-CA-C	5.32	116.87	107.61
1	A	261	PRO	O-C-N	5.12	123.67	121.31
1	A	258	PHE	N-CA-C	5.08	116.96	108.99
1	D	258	PHE	N-CA-C	5.04	117.05	109.23

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	2172	0	2114	48	0
1	B	2172	0	2114	56	0
1	C	2172	0	2114	51	0
1	D	2172	0	2114	49	0
2	A	5	0	0	0	0
2	B	15	0	0	7	0
2	C	15	0	0	4	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	8732	0	8456	198	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 12.

All (198) 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:247:ILE:O	1:C:247:ILE:HD12	1.47	1.15
1:C:50:ASN:HB2	1:C:52:GLN:NE2	1.63	1.13
1:D:108:MSE:HE2	1:D:113:ILE:HG13	1.28	1.10
1:D:108:MSE:HE1	1:D:113:ILE:HA	1.41	1.01
1:D:199:ILE:O	1:D:203:GLN:HG2	1.63	0.99
1:B:50:ASN:HB2	1:B:52:GLN:HE22	1.26	0.98
1:C:176:HIS:HB3	2:C:302:PO4:O2	1.64	0.96
1:B:108:MSE:HE3	1:B:112:GLU:HB3	1.48	0.95
1:C:50:ASN:HB2	1:C:52:GLN:HE22	1.19	0.93
1:C:82:SER:OG	1:C:85:GLN:HG3	1.74	0.88
1:D:108:MSE:HE2	1:D:113:ILE:CG1	2.06	0.84
1:C:50:ASN:CB	1:C:52:GLN:NE2	2.42	0.83
1:D:50:ASN:HB2	1:D:52:GLN:NE2	1.94	0.83
1:D:40:MSE:HG3	1:D:73:THR:HG23	1.64	0.80
1:B:181:ARG:NH2	2:B:300:PO4:O1	2.14	0.79
1:A:50:ASN:HB2	1:A:52:GLN:NE2	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASN:CB	1:A:52:GLN:HE22	1.97	0.78
1:A:50:ASN:HB2	1:A:52:GLN:HE22	1.47	0.78
1:C:61:TYR:HB2	1:C:171:ILE:HG12	1.67	0.76
1:C:50:ASN:CB	1:C:52:GLN:HE22	1.99	0.75
1:D:108:MSE:CE	1:D:113:ILE:HG13	2.14	0.74
1:B:108:MSE:HE1	1:B:113:ILE:HA	1.71	0.73
1:A:108:MSE:HE2	1:A:112:GLU:HB3	1.72	0.72
1:A:197:GLU:HG2	1:C:140:THR:CB	2.21	0.71
1:B:181:ARG:NH1	2:B:300:PO4:O1	2.23	0.70
1:C:268:HIS:ND1	2:C:272:PO4:O2	2.25	0.70
1:D:108:MSE:CE	1:D:113:ILE:HA	2.19	0.69
1:A:50:ASN:CB	1:A:52:GLN:NE2	2.55	0.69
1:B:69:ARG:NH2	2:B:302:PO4:O3	2.23	0.69
1:A:197:GLU:HG2	1:C:140:THR:HB	1.74	0.69
1:C:193:GLN:HE21	1:C:220:SER:HB2	1.58	0.69
1:A:101:GLU:HB2	1:A:139:GLU:HG3	1.76	0.68
1:B:157:ASN:OD1	1:B:161:LYS:HE2	1.94	0.67
1:D:50:ASN:CB	1:D:52:GLN:NE2	2.57	0.67
1:D:40:MSE:HE1	1:D:235:GLY:HA2	1.76	0.67
1:A:23:GLN:HG2	1:A:107:GLY:O	1.94	0.67
1:D:108:MSE:HE1	1:D:113:ILE:CA	2.21	0.66
1:C:101:GLU:HB2	1:C:139:GLU:HG3	1.78	0.66
1:B:16:THR:HG21	1:B:69:ARG:HD2	1.79	0.65
1:A:197:GLU:HG2	1:C:140:THR:CG2	2.27	0.64
1:A:197:GLU:HG2	1:C:140:THR:HG21	1.80	0.64
1:C:268:HIS:HB2	2:C:272:PO4:O2	1.97	0.64
1:B:62:ILE:HG12	1:B:172:MSE:HB2	1.80	0.64
1:A:268:HIS:HB2	2:B:300:PO4:O2	1.98	0.63
1:B:156:GLN:HG2	1:B:242:TYR:OH	1.99	0.62
1:D:61:TYR:HB2	1:D:171:ILE:HG12	1.82	0.62
1:C:40:MSE:HG3	1:C:73:THR:HG23	1.80	0.62
1:D:67:ARG:NE	1:D:67:ARG:HA	2.15	0.62
1:B:40:MSE:HG3	1:B:73:THR:HG23	1.82	0.61
1:C:242:TYR:CD1	1:C:247:ILE:HA	2.35	0.61
1:C:247:ILE:HD12	1:C:247:ILE:C	2.24	0.61
1:C:108:MSE:HE3	1:C:112:GLU:HB3	1.82	0.60
1:D:67:ARG:HA	1:D:67:ARG:HE	1.67	0.60
1:A:18:TRP:CG	1:A:30:LEU:HD11	2.37	0.60
1:D:108:MSE:CE	1:D:113:ILE:CA	2.79	0.59
1:B:50:ASN:HB2	1:B:52:GLN:NE2	2.08	0.59
1:B:40:MSE:HE2	1:B:73:THR:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:HG2	1:A:76:LEU:HD11	1.85	0.58
1:B:253:GLU:HG2	1:B:255:ALA:HB2	1.86	0.58
1:A:233:ASP:OD1	1:A:234:ALA:N	2.37	0.57
1:A:148:LEU:O	1:A:152:ILE:HG13	2.05	0.57
1:A:150:ARG:HG3	1:A:218:LEU:HD11	1.86	0.57
1:D:52:GLN:HB2	1:D:258:PHE:HB3	1.86	0.57
1:A:242:TYR:CD1	1:A:247:ILE:HA	2.39	0.57
1:D:108:MSE:CE	1:D:113:ILE:N	2.68	0.57
1:A:16:THR:HG21	1:A:69:ARG:HD2	1.86	0.56
1:A:40:MSE:HG3	1:A:73:THR:HG23	1.87	0.56
1:D:10:ILE:HB	1:D:180:LEU:HD13	1.87	0.56
1:C:108:MSE:HE1	1:C:112:GLU:C	2.31	0.56
1:D:242:TYR:CE1	1:D:247:ILE:HD12	2.41	0.56
1:B:181:ARG:CZ	2:B:300:PO4:O1	2.53	0.56
1:C:40:MSE:HE1	1:C:235:GLY:HA2	1.88	0.55
1:B:247:ILE:HG13	1:B:247:ILE:O	2.05	0.55
1:A:186:ILE:O	1:A:187:TRP:C	2.50	0.54
1:C:50:ASN:HB2	1:C:52:GLN:HE21	1.68	0.54
1:B:61:TYR:HB2	1:B:171:ILE:HG12	1.89	0.54
1:C:253:GLU:HG2	1:C:255:ALA:HB2	1.90	0.54
1:D:16:THR:HG21	1:D:69:ARG:HD2	1.89	0.53
1:A:24:TYR:N	1:A:24:TYR:CD1	2.76	0.53
1:C:108:MSE:HE2	1:C:113:ILE:HG13	1.91	0.53
1:D:4:LEU:HD23	1:D:262:PRO:HD3	1.90	0.53
1:B:242:TYR:CD1	1:B:247:ILE:HA	2.43	0.52
1:B:270:ASP:C	1:B:271:VAL:HG23	2.34	0.52
1:B:242:TYR:CZ	1:B:247:ILE:HD12	2.44	0.52
1:B:186:ILE:O	1:B:187:TRP:C	2.50	0.52
1:B:108:MSE:CE	1:B:113:ILE:N	2.72	0.52
1:D:48:PHE:CE1	1:D:54:LEU:HD13	2.45	0.52
1:B:56:PRO:HA	1:B:59:ILE:HG13	1.91	0.52
1:A:52:GLN:HB2	1:A:258:PHE:HB3	1.91	0.52
1:B:18:TRP:CZ3	1:B:107:GLY:HA2	2.45	0.51
1:B:157:ASN:HD21	1:B:214:PRO:HG2	1.75	0.51
1:C:232:LEU:HD12	1:C:236:GLY:HA3	1.92	0.51
1:C:159:HIS:CD2	1:C:171:ILE:HD12	2.46	0.51
1:A:50:ASN:HB3	1:A:52:GLN:HE22	1.72	0.50
1:D:198:THR:OG1	1:D:201:GLU:HG3	2.11	0.50
1:B:139:GLU:HA	1:B:143:GLN:OE1	2.11	0.50
1:D:132:ARG:HB2	1:D:225:VAL:O	2.12	0.50
1:D:94:ASP:OD1	1:D:96:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLY:HA2	1:B:237:ILE:HG13	1.92	0.49
1:B:157:ASN:ND2	1:B:214:PRO:HG2	2.27	0.49
1:A:10:ILE:HG22	1:A:173:VAL:HB	1.94	0.49
1:B:18:TRP:CG	1:B:30:LEU:HD11	2.48	0.49
1:C:108:MSE:HE3	1:C:112:GLU:CB	2.43	0.49
1:B:108:MSE:CE	1:B:112:GLU:C	2.86	0.49
1:B:140:THR:OG1	1:B:143:GLN:HG3	2.12	0.49
1:C:18:TRP:CG	1:C:30:LEU:HD11	2.48	0.49
1:B:148:LEU:HD13	1:B:182:TYR:HB3	1.95	0.49
1:C:67:ARG:NE	1:C:67:ARG:HA	2.28	0.48
1:C:176:HIS:CB	2:C:302:PO4:O2	2.50	0.48
1:C:247:ILE:O	1:C:247:ILE:CD1	2.39	0.48
1:C:105:TYR:O	1:C:106:GLU:C	2.57	0.48
1:B:108:MSE:CE	1:B:113:ILE:HA	2.42	0.48
1:D:50:ASN:CB	1:D:52:GLN:HE21	2.27	0.47
1:D:99:GLU:OE1	1:D:178:HIS:HB2	2.14	0.47
1:A:239:VAL:HG12	1:A:253:GLU:HB3	1.97	0.47
1:D:18:TRP:CZ3	1:D:107:GLY:HA2	2.49	0.47
1:B:176:HIS:ND1	2:B:302:PO4:O3	2.48	0.47
1:D:61:TYR:O	1:D:171:ILE:HA	2.15	0.46
1:A:196:CYS:HB3	1:A:201:GLU:O	2.14	0.46
1:C:94:ASP:OD1	1:C:96:ASP:HB2	2.15	0.46
1:D:159:HIS:CD2	1:D:171:ILE:HD12	2.51	0.46
1:C:233:ASP:OD1	1:C:234:ALA:N	2.49	0.46
1:D:261:PRO:HB2	1:D:263:GLU:OE1	2.15	0.46
1:B:67:ARG:HG3	1:B:69:ARG:NH1	2.31	0.46
1:D:105:TYR:OH	1:D:136:GLU:OE1	2.30	0.45
1:C:5:THR:OG1	1:C:245:HIS:ND1	2.49	0.45
1:B:52:GLN:HB2	1:B:258:PHE:HB3	1.98	0.45
1:C:50:ASN:CB	1:C:52:GLN:HE21	2.26	0.45
1:C:99:GLU:OE1	1:C:178:HIS:HB2	2.16	0.45
1:A:263:GLU:HG2	1:A:264:GLU:HG2	1.98	0.45
1:D:270:ASP:C	1:D:271:VAL:HG23	2.41	0.45
1:A:81:LEU:HD12	1:A:81:LEU:N	2.32	0.45
1:D:105:TYR:O	1:D:106:GLU:C	2.58	0.45
1:D:124:LYS:HD2	1:D:124:LYS:HA	1.87	0.45
1:C:156:GLN:HG2	1:C:242:TYR:OH	2.17	0.45
1:A:270:ASP:C	1:A:271:VAL:HG23	2.43	0.44
1:A:108:MSE:HE2	1:A:112:GLU:CB	2.45	0.44
1:D:247:ILE:O	1:D:247:ILE:HG13	2.15	0.44
1:B:67:ARG:HH21	1:B:67:ARG:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:GLN:HB2	1:C:258:PHE:HB3	1.99	0.44
1:A:50:ASN:HB3	1:A:52:GLN:NE2	2.32	0.44
1:C:239:VAL:HG12	1:C:253:GLU:HB3	1.99	0.44
1:D:246:ASN:OD1	1:D:248:ASP:HB2	2.17	0.44
1:A:212:THR:O	1:A:214:PRO:HD3	2.17	0.44
1:B:148:LEU:CD1	1:B:182:TYR:HB3	2.48	0.44
1:D:252:LEU:C	1:D:252:LEU:HD23	2.42	0.43
1:A:140:THR:HG23	1:A:143:GLN:OE1	2.18	0.43
1:B:108:MSE:HE3	1:B:112:GLU:CB	2.35	0.43
1:A:99:GLU:HA	1:A:99:GLU:OE1	2.18	0.43
1:B:159:HIS:CD2	1:B:171:ILE:HD12	2.54	0.43
1:B:108:MSE:HE1	1:B:113:ILE:CA	2.44	0.43
1:A:61:TYR:O	1:A:171:ILE:HA	2.18	0.43
1:B:38:GLY:O	1:B:42:ARG:HG3	2.18	0.43
1:D:228:PRO:HB2	1:D:230:PHE:CD2	2.54	0.43
1:C:270:ASP:O	1:C:271:VAL:HB	2.18	0.43
1:A:137:ASN:ND2	1:C:124:LYS:HE3	2.34	0.42
1:B:40:MSE:HE2	1:B:73:THR:HG21	2.00	0.42
1:C:24:TYR:CD1	1:C:24:TYR:N	2.87	0.42
1:D:108:MSE:HE3	1:D:112:GLU:C	2.44	0.42
1:A:244:HIS:H	1:A:267:GLN:NE2	2.17	0.42
1:C:196:CYS:HB3	1:C:201:GLU:O	2.18	0.42
1:B:242:TYR:CE1	1:B:247:ILE:HD12	2.54	0.42
1:A:28:THR:OG1	1:A:106:GLU:OE2	2.36	0.42
1:A:129:ASN:OD1	1:A:129:ASN:C	2.63	0.42
1:B:8:CYS:HA	1:B:171:ILE:O	2.20	0.42
1:C:61:TYR:O	1:C:171:ILE:HA	2.19	0.42
1:A:24:TYR:N	1:A:24:TYR:HD1	2.17	0.42
1:A:156:GLN:HG2	1:A:242:TYR:OH	2.18	0.42
1:A:50:ASN:O	1:A:51:ASN:HB2	2.20	0.42
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.89	0.42
1:D:108:MSE:HE3	1:D:113:ILE:N	2.34	0.42
1:B:241:SER:OG	1:B:242:TYR:N	2.52	0.42
1:D:186:ILE:O	1:D:187:TRP:C	2.63	0.42
1:B:200:GLU:H	1:B:200:GLU:CD	2.27	0.41
1:A:268:HIS:ND1	2:B:300:PO4:O2	2.51	0.41
1:D:13:HIS:CG	1:D:69:ARG:HG3	2.55	0.41
1:B:50:ASN:O	1:B:51:ASN:HB2	2.20	0.41
1:D:40:MSE:CE	1:D:235:GLY:HA2	2.47	0.41
1:D:248:ASP:O	1:D:250:PRO:HD3	2.20	0.41
1:B:199:ILE:H	1:B:199:ILE:HG12	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:C	1:C:252:LEU:HD23	2.46	0.41
1:B:270:ASP:OD1	1:B:271:VAL:N	2.53	0.41
1:C:62:ILE:HD12	1:C:89:ILE:HG21	2.03	0.41
1:D:18:TRP:CG	1:D:30:LEU:HD11	2.55	0.41
1:D:152:ILE:CD1	1:D:186:ILE:HG13	2.51	0.41
1:D:222:ARG:HG3	1:D:222:ARG:NH2	2.36	0.41
1:A:180:LEU:HD23	1:A:180:LEU:HA	1.88	0.41
1:B:246:ASN:OD1	1:B:248:ASP:HB2	2.21	0.41
1:C:48:PHE:O	1:C:49:ARG:C	2.63	0.41
1:C:244:HIS:H	1:C:267:GLN:HE22	1.69	0.41
1:A:144:ILE:HG23	1:A:182:TYR:CE2	2.54	0.40
1:C:210:ASP:OD1	1:C:210:ASP:C	2.64	0.40
1:D:248:ASP:C	1:D:250:PRO:HD3	2.45	0.40
1:B:94:ASP:O	1:B:97:LEU:HB2	2.21	0.40
1:B:10:ILE:HB	1:B:180:LEU:HD13	2.03	0.40
1:B:24:TYR:HD2	1:B:102:TYR:CE1	2.39	0.40
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.87	0.40
1:B:270:ASP:O	1:B:271:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	267/292 (91%)	257 (96%)	10 (4%)	0	100	100
1	B	267/292 (91%)	257 (96%)	8 (3%)	2 (1%)	18	38
1	C	267/292 (91%)	255 (96%)	11 (4%)	1 (0%)	30	51
1	D	267/292 (91%)	258 (97%)	7 (3%)	2 (1%)	18	38
All	All	1068/1168 (91%)	1027 (96%)	36 (3%)	5 (0%)	24	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	206	LYS
1	B	175	ALA
1	B	241	SER
1	D	175	ALA
1	C	241	SER

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	235/250 (94%)	217 (92%)	18 (8%)	12	27
1	B	235/250 (94%)	212 (90%)	23 (10%)	7	17
1	C	235/250 (94%)	220 (94%)	15 (6%)	16	35
1	D	235/250 (94%)	218 (93%)	17 (7%)	13	30
All	All	940/1000 (94%)	867 (92%)	73 (8%)	11	26

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	45	GLU
1	A	49	ARG
1	A	52	GLN
1	A	54	LEU
1	A	59	ILE
1	A	65	SER
1	A	126	ARG
1	A	142	GLN
1	A	188	PHE
1	A	192	VAL
1	A	197	GLU
1	A	222	ARG
1	A	231	LEU
1	A	241	SER
1	A	247	ILE
1	A	265	GLU

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Mol	Chain	Res	Type
1	A	266	SER
1	B	17	GLU
1	B	25	THR
1	B	45	GLU
1	B	49	ARG
1	B	52	GLN
1	B	54	LEU
1	B	67	ARG
1	B	91	VAL
1	B	111	ARG
1	B	118	LYS
1	B	126	ARG
1	B	164	SER
1	B	186	ILE
1	B	188	PHE
1	B	190	LEU
1	B	192	VAL
1	B	194	LYS
1	B	199	ILE
1	B	205	VAL
1	B	217	LYS
1	B	231	LEU
1	B	247	ILE
1	B	271	VAL
1	C	9	ILE
1	C	10	ILE
1	C	17	GLU
1	C	52	GLN
1	C	54	LEU
1	C	115	GLU
1	C	130	ILE
1	C	186	ILE
1	C	192	VAL
1	C	198	THR
1	C	220	SER
1	C	231	LEU
1	C	247	ILE
1	C	259	VAL
1	C	262	PRO
1	D	17	GLU
1	D	52	GLN
1	D	54	LEU

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Mol	Chain	Res	Type
1	D	115	GLU
1	D	118	LYS
1	D	125	GLU
1	D	126	ARG
1	D	142	GLN
1	D	164	SER
1	D	186	ILE
1	D	199	ILE
1	D	203	GLN
1	D	205	VAL
1	D	217	LYS
1	D	231	LEU
1	D	247	ILE
1	D	263	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	137	ASN
1	A	203	GLN
1	A	204	ASN
1	A	267	GLN
1	B	23	GLN
1	B	52	GLN
1	B	137	ASN
1	B	267	GLN
1	C	15	GLN
1	C	23	GLN
1	C	52	GLN
1	C	58	ASN
1	C	137	ASN
1	C	157	ASN
1	C	203	GLN
1	C	267	GLN
1	D	52	GLN
1	D	137	ASN
1	D	142	GLN
1	D	193	GLN
1	D	267	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 oligosaccharides 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	C	272	-	4,4,4	1.52	1 (25%)	6,6,6	2.08	2 (33%)
2	PO4	D	302	-	4,4,4	1.02	0	6,6,6	1.95	2 (33%)
2	PO4	B	302	-	4,4,4	0.68	0	6,6,6	1.55	2 (33%)
2	PO4	C	300	-	4,4,4	0.70	0	6,6,6	2.60	3 (50%)
2	PO4	B	300	-	4,4,4	0.92	0	6,6,6	1.93	2 (33%)
2	PO4	C	302	-	4,4,4	1.59	1 (25%)	6,6,6	0.67	0
2	PO4	B	272	-	4,4,4	0.88	0	6,6,6	1.41	2 (33%)
2	PO4	A	302	-	4,4,4	0.88	0	6,6,6	1.35	1 (16%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	272	PO4	P-O2	-2.33	1.47	1.54
2	C	302	PO4	P-O3	-2.02	1.48	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	PO4	O4-P-O3	4.38	121.53	107.91
2	C	272	PO4	O2-P-O1	-4.02	96.74	110.95
2	C	300	PO4	O4-P-O1	-3.21	99.61	110.95
2	D	302	PO4	O3-P-O1	-3.09	100.04	110.95
2	B	300	PO4	O2-P-O1	-2.85	100.88	110.95
2	B	300	PO4	O4-P-O3	2.74	116.44	107.91
2	D	302	PO4	O2-P-O1	2.73	120.62	110.95
2	B	302	PO4	O4-P-O1	-2.59	101.81	110.95
2	A	302	PO4	O4-P-O2	2.58	115.95	107.91
2	C	272	PO4	O4-P-O1	2.50	119.80	110.95
2	C	300	PO4	O3-P-O2	-2.39	100.47	107.91
2	B	272	PO4	O3-P-O1	-2.36	102.61	110.95
2	B	272	PO4	O4-P-O3	2.16	114.62	107.91
2	B	302	PO4	O4-P-O2	2.08	114.40	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	272	PO4	2	0
2	B	302	PO4	2	0
2	B	300	PO4	5	0
2	C	302	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 [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	266/292 (91%)	0.01	3 (1%) 78 74	14, 24, 41, 56	0
1	B	266/292 (91%)	0.06	2 (0%) 82 80	14, 24, 41, 56	0
1	C	266/292 (91%)	0.06	4 (1%) 72 68	14, 24, 41, 56	0
1	D	266/292 (91%)	0.03	4 (1%) 72 68	14, 24, 41, 55	0
All	All	1064/1168 (91%)	0.04	13 (1%) 76 73	14, 24, 43, 56	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	VAL	3.2
1	C	121	GLY	3.1
1	A	199	ILE	3.0
1	C	271	VAL	2.7
1	A	197	GLU	2.6
1	A	200	GLU	2.6
1	D	263	GLU	2.6
1	B	125	GLU	2.6
1	D	200	GLU	2.5
1	C	263	GLU	2.4
1	D	199	ILE	2.2
1	C	200	GLU	2.1
1	D	198	THR	2.1

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	300	5/5	0.79	0.12	32,37,42,43	0
2	PO4	B	272	5/5	0.92	0.08	27,27,29,29	0
2	PO4	B	302	5/5	0.94	0.10	16,24,25,27	0
2	PO4	C	300	5/5	0.94	0.08	14,15,19,21	0
2	PO4	C	272	5/5	0.94	0.09	22,22,22,22	0
2	PO4	D	302	5/5	0.96	0.07	4,9,15,18	0
2	PO4	A	302	5/5	0.97	0.09	15,22,23,24	0
2	PO4	C	302	5/5	0.99	0.05	2,5,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.