



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:24 PM UTC

PDB ID : 4UPH / pdb_00004uph
Title : Crystal Structure of Phosphonate Monoester Hydrolase of *Agrobacterium radiobacter*
Authors : Fischer, G.; Loo, B.v.; Hyvonen, M.; Hollfelder, F.
Deposited on : 2014-06-17
Resolution : 2.50 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)
Xtrriage (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

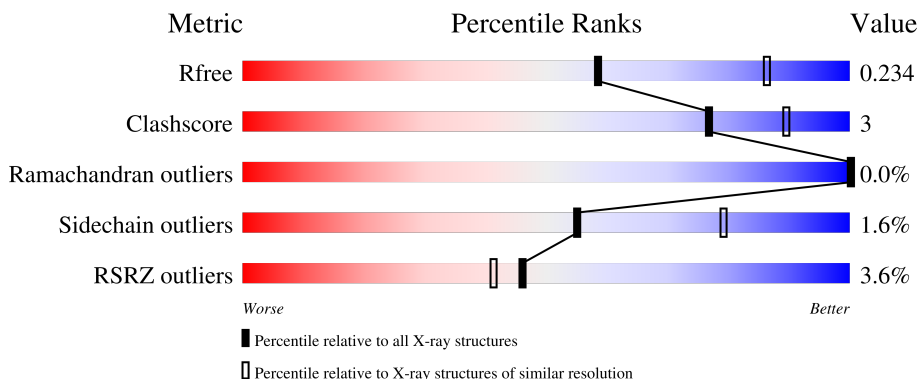
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	547	 83% 9% 8%
1	B	547	 83% 8% 8%
1	C	547	 82% 9% 8%
1	D	547	 82% 9% 8%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16052 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 SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	504	3926	2495	688	731	12	0	0	0
1	B	504	3926	2495	688	731	12	0	0	0
1	C	504	3926	2495	688	731	12	0	0	0
1	D	504	3926	2495	688	731	12	0	0	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	MET	-	expression tag	UNP B9JE48
A	-27	ALA	-	expression tag	UNP B9JE48
A	-26	SER	-	expression tag	UNP B9JE48
A	-25	TRP	-	expression tag	UNP B9JE48
A	-24	SER	-	expression tag	UNP B9JE48
A	-23	HIS	-	expression tag	UNP B9JE48
A	-22	PRO	-	expression tag	UNP B9JE48
A	-21	GLN	-	expression tag	UNP B9JE48
A	-20	PHE	-	expression tag	UNP B9JE48
A	-19	GLU	-	expression tag	UNP B9JE48
A	-18	LYS	-	expression tag	UNP B9JE48
A	-17	GLY	-	expression tag	UNP B9JE48
A	-16	ALA	-	expression tag	UNP B9JE48
A	-15	GLU	-	expression tag	UNP B9JE48
A	-14	THR	-	expression tag	UNP B9JE48
A	-13	ALA	-	expression tag	UNP B9JE48
A	-12	VAL	-	expression tag	UNP B9JE48
A	-11	PRO	-	expression tag	UNP B9JE48
A	-10	ASN	-	expression tag	UNP B9JE48
A	-9	SER	-	expression tag	UNP B9JE48
A	-8	SER	-	expression tag	UNP B9JE48

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	SER	-	expression tag	UNP B9JE48
A	-6	VAL	-	expression tag	UNP B9JE48
A	-5	PRO	-	expression tag	UNP B9JE48
A	-4	GLY	-	expression tag	UNP B9JE48
A	-3	ASP	-	expression tag	UNP B9JE48
A	-2	PRO	-	expression tag	UNP B9JE48
A	-1	SER	-	expression tag	UNP B9JE48
A	0	SER	-	expression tag	UNP B9JE48
B	-28	MET	-	expression tag	UNP B9JE48
B	-27	ALA	-	expression tag	UNP B9JE48
B	-26	SER	-	expression tag	UNP B9JE48
B	-25	TRP	-	expression tag	UNP B9JE48
B	-24	SER	-	expression tag	UNP B9JE48
B	-23	HIS	-	expression tag	UNP B9JE48
B	-22	PRO	-	expression tag	UNP B9JE48
B	-21	GLN	-	expression tag	UNP B9JE48
B	-20	PHE	-	expression tag	UNP B9JE48
B	-19	GLU	-	expression tag	UNP B9JE48
B	-18	LYS	-	expression tag	UNP B9JE48
B	-17	GLY	-	expression tag	UNP B9JE48
B	-16	ALA	-	expression tag	UNP B9JE48
B	-15	GLU	-	expression tag	UNP B9JE48
B	-14	THR	-	expression tag	UNP B9JE48
B	-13	ALA	-	expression tag	UNP B9JE48
B	-12	VAL	-	expression tag	UNP B9JE48
B	-11	PRO	-	expression tag	UNP B9JE48
B	-10	ASN	-	expression tag	UNP B9JE48
B	-9	SER	-	expression tag	UNP B9JE48
B	-8	SER	-	expression tag	UNP B9JE48
B	-7	SER	-	expression tag	UNP B9JE48
B	-6	VAL	-	expression tag	UNP B9JE48
B	-5	PRO	-	expression tag	UNP B9JE48
B	-4	GLY	-	expression tag	UNP B9JE48
B	-3	ASP	-	expression tag	UNP B9JE48
B	-2	PRO	-	expression tag	UNP B9JE48
B	-1	SER	-	expression tag	UNP B9JE48
B	0	SER	-	expression tag	UNP B9JE48
C	-28	MET	-	expression tag	UNP B9JE48
C	-27	ALA	-	expression tag	UNP B9JE48
C	-26	SER	-	expression tag	UNP B9JE48
C	-25	TRP	-	expression tag	UNP B9JE48
C	-24	SER	-	expression tag	UNP B9JE48

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-23	HIS	-	expression tag	UNP B9JE48
C	-22	PRO	-	expression tag	UNP B9JE48
C	-21	GLN	-	expression tag	UNP B9JE48
C	-20	PHE	-	expression tag	UNP B9JE48
C	-19	GLU	-	expression tag	UNP B9JE48
C	-18	LYS	-	expression tag	UNP B9JE48
C	-17	GLY	-	expression tag	UNP B9JE48
C	-16	ALA	-	expression tag	UNP B9JE48
C	-15	GLU	-	expression tag	UNP B9JE48
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C	-11	PRO	-	expression tag	UNP B9JE48
C	-10	ASN	-	expression tag	UNP B9JE48
C	-9	SER	-	expression tag	UNP B9JE48
C	-8	SER	-	expression tag	UNP B9JE48
C	-7	SER	-	expression tag	UNP B9JE48
C	-6	VAL	-	expression tag	UNP B9JE48
C	-5	PRO	-	expression tag	UNP B9JE48
C	-4	GLY	-	expression tag	UNP B9JE48
C	-3	ASP	-	expression tag	UNP B9JE48
C	-2	PRO	-	expression tag	UNP B9JE48
C	-1	SER	-	expression tag	UNP B9JE48
C	0	SER	-	expression tag	UNP B9JE48
D	-28	MET	-	expression tag	UNP B9JE48
D	-27	ALA	-	expression tag	UNP B9JE48
D	-26	SER	-	expression tag	UNP B9JE48
D	-25	TRP	-	expression tag	UNP B9JE48
D	-24	SER	-	expression tag	UNP B9JE48
D	-23	HIS	-	expression tag	UNP B9JE48
D	-22	PRO	-	expression tag	UNP B9JE48
D	-21	GLN	-	expression tag	UNP B9JE48
D	-20	PHE	-	expression tag	UNP B9JE48
D	-19	GLU	-	expression tag	UNP B9JE48
D	-18	LYS	-	expression tag	UNP B9JE48
D	-17	GLY	-	expression tag	UNP B9JE48
D	-16	ALA	-	expression tag	UNP B9JE48
D	-15	GLU	-	expression tag	UNP B9JE48
D	-14	THR	-	expression tag	UNP B9JE48
D	-13	ALA	-	expression tag	UNP B9JE48
D	-12	VAL	-	expression tag	UNP B9JE48
D	-11	PRO	-	expression tag	UNP B9JE48

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-10	ASN	-	expression tag	UNP B9JE48
D	-9	SER	-	expression tag	UNP B9JE48
D	-8	SER	-	expression tag	UNP B9JE48
D	-7	SER	-	expression tag	UNP B9JE48
D	-6	VAL	-	expression tag	UNP B9JE48
D	-5	PRO	-	expression tag	UNP B9JE48
D	-4	GLY	-	expression tag	UNP B9JE48
D	-3	ASP	-	expression tag	UNP B9JE48
D	-2	PRO	-	expression tag	UNP B9JE48
D	-1	SER	-	expression tag	UNP B9JE48
D	0	SER	-	expression tag	UNP B9JE48

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	121	Total O 121 121	0	0

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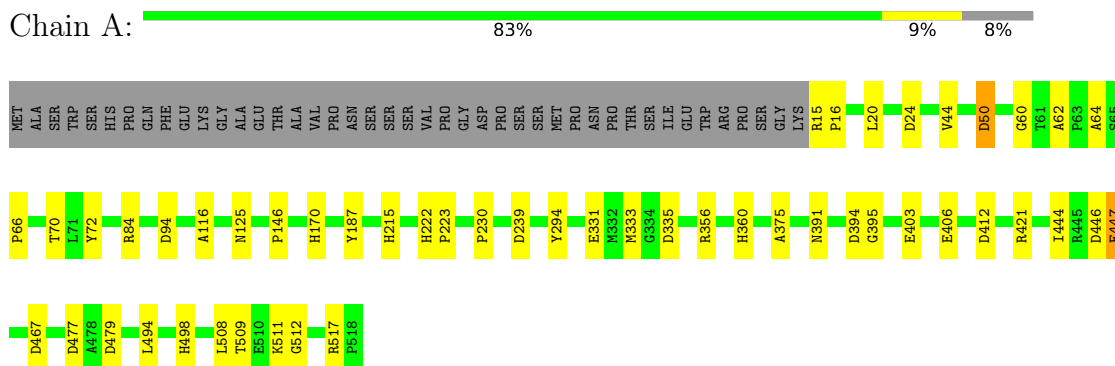
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	84	Total O 84 84	0	0
4	C	81	Total O 81 81	0	0
4	D	54	Total O 54 54	0	0

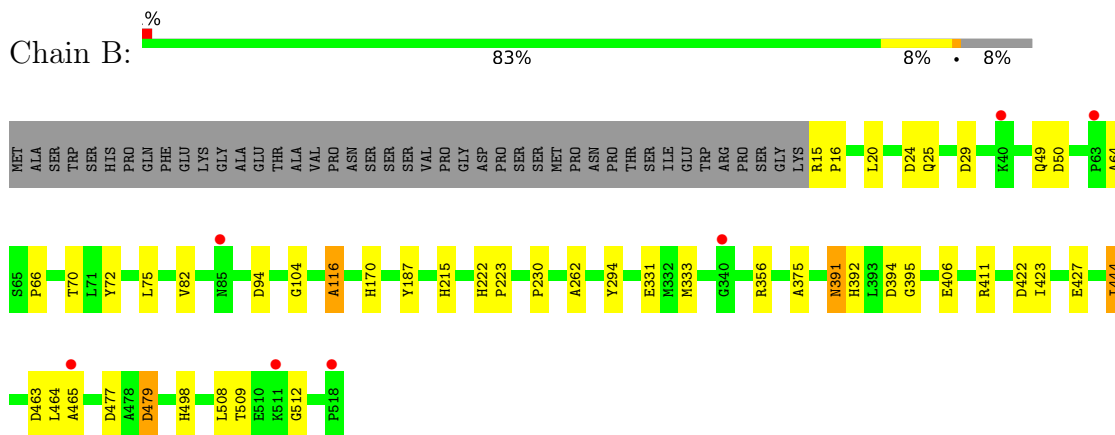
3 Residue-property plots [i](#)

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.

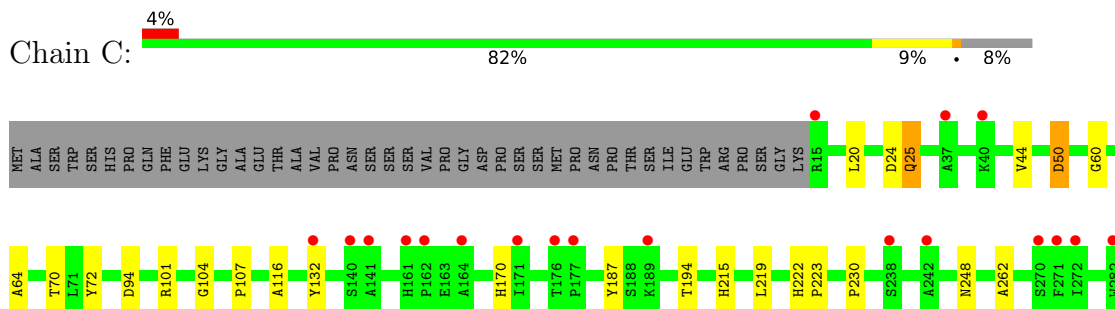
- Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN



- Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN

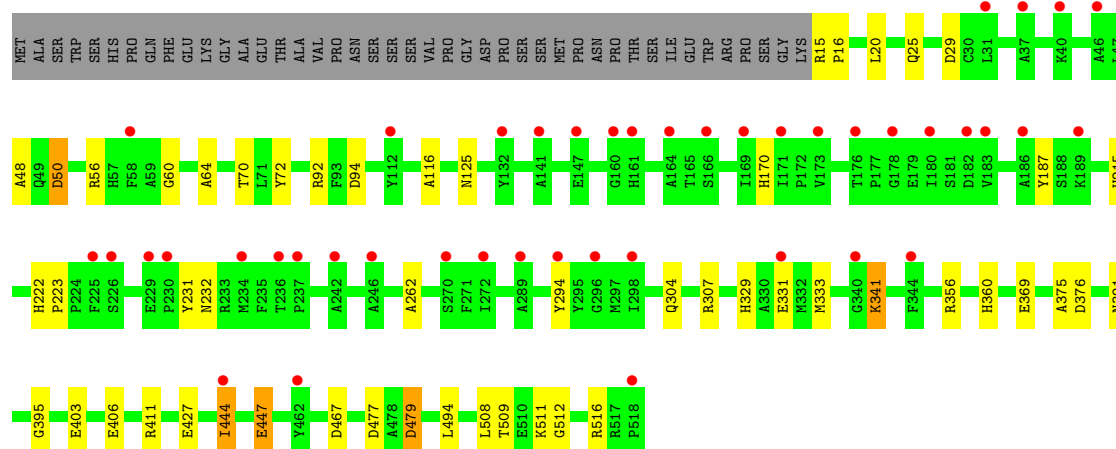
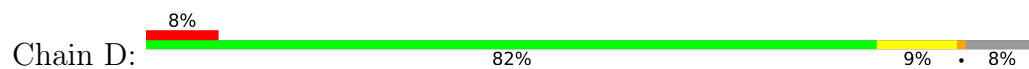


- Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN





● Molecule 1: SULFATASE (SULFURIC ESTER HYDROLASE) PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	232.69Å 232.69Å 112.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.17 – 2.50 58.17 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.17-2.50) 100.0 (58.17-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.51Å)	Xtrriage
Refinement program	BUSTER 2.10.1	Depositor
R, R_{free}	0.196 , 0.225 0.207 , 0.234	Depositor DCC
R_{free} test set	5295 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtrriage
Anisotropy	0.398	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16052	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 22.35 % 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 5.7999e-03. 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: MG, CL, DDZ

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	0.87	1/4037 (0.0%)	1.28	14/5503 (0.3%)
1	B	0.86	0/4037	1.30	11/5503 (0.2%)
1	C	0.85	0/4037	1.29	15/5503 (0.3%)
1	D	0.86	0/4037	1.30	8/5503 (0.1%)
All	All	0.86	1/16148 (0.0%)	1.29	48/22012 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	ALA	CA-C	5.31	1.58	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ASP	CA-CB-CG	7.39	119.99	112.60
1	D	467	ASP	CA-CB-CG	6.17	118.77	112.60
1	C	446	ASP	CA-CB-CG	5.99	118.59	112.60
1	C	335	ASP	CA-CB-CG	5.97	118.57	112.60
1	A	335	ASP	CA-CB-CG	5.93	118.53	112.60
1	D	48	ALA	CA-C-N	5.89	128.45	120.38
1	D	48	ALA	C-N-CA	5.89	128.45	120.38
1	D	232	ASN	CA-CB-CG	5.89	118.49	112.60
1	A	467	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	230	PRO	CA-C-N	5.59	128.54	120.38
1	C	230	PRO	C-N-CA	5.59	128.54	120.38
1	A	230	PRO	CA-C-N	5.54	128.46	120.38
1	A	230	PRO	C-N-CA	5.54	128.46	120.38
1	C	479	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	230	PRO	CA-C-N	5.50	128.41	120.38
1	B	230	PRO	C-N-CA	5.50	128.41	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ASP	CA-CB-CG	5.48	118.08	112.60
1	C	248	ASN	CA-C-N	5.48	127.89	120.38
1	C	248	ASN	C-N-CA	5.48	127.89	120.38
1	B	391	ASN	CA-C-N	5.46	128.59	120.90
1	B	391	ASN	C-N-CA	5.46	128.59	120.90
1	C	467	ASP	CA-CB-CG	5.33	117.93	112.60
1	D	262	ALA	N-CA-C	5.33	117.17	111.36
1	C	346	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	44	VAL	N-CA-C	-5.30	105.55	110.53
1	D	444	ILE	N-CA-CB	5.30	118.58	111.90
1	C	132	TYR	N-CA-C	-5.29	106.88	113.38
1	A	146	PRO	CA-C-N	5.25	127.57	120.38
1	A	146	PRO	C-N-CA	5.25	127.57	120.38
1	B	444	ILE	N-CA-CB	5.25	118.51	111.90
1	B	262	ALA	N-CA-C	5.25	117.08	111.36
1	B	479	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	412	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	44	VAL	N-CA-C	-5.16	105.68	110.53
1	B	464	LEU	CA-C-N	5.14	127.12	120.44
1	B	464	LEU	C-N-CA	5.14	127.12	120.44
1	D	29	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	262	ALA	N-CA-C	5.11	116.93	111.36
1	C	328	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	116	ALA	N-CA-C	-5.08	103.25	109.65
1	C	444	ILE	N-CA-CB	5.07	118.29	111.90
1	D	479	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	477	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	66	PRO	CA-C-N	5.05	127.47	120.29
1	A	66	PRO	C-N-CA	5.05	127.47	120.29
1	B	29	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	239	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	477	ASP	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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	3926	0	3741	21	0
1	B	3926	0	3741	26	0
1	C	3926	0	3741	24	0
1	D	3926	0	3741	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	121	0	0	1	0
4	B	84	0	0	2	0
4	C	81	0	0	0	0
4	D	54	0	0	1	0
All	All	16052	0	14964	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (90) 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:94:ASP:H	1:B:391:ASN:HD21	1.24	0.86
1:A:94:ASP:H	1:A:391:ASN:HD21	1.25	0.82
1:D:94:ASP:H	1:D:391:ASN:HD21	1.24	0.81
1:B:509:THR:HG22	1:B:512:GLY:O	1.83	0.79
1:A:84:ARG:HD2	1:A:421:ARG:O	1.83	0.79
1:C:509:THR:HG22	1:C:512:GLY:O	1.85	0.76
1:A:509:THR:HG22	1:A:512:GLY:O	1.86	0.75
1:C:94:ASP:H	1:C:391:ASN:HD21	1.33	0.74
1:D:509:THR:HG22	1:D:512:GLY:O	1.88	0.72
1:A:447:GLU:H	1:A:447:GLU:CD	2.03	0.66
1:B:15:ARG:HB3	1:B:16:PRO:HD3	1.78	0.65
1:C:329:HIS:CE1	1:C:341:LYS:HD2	2.31	0.65
1:D:60:GLY:HA3	1:D:70:THR:HG21	1.79	0.62
1:D:447:GLU:H	1:D:447:GLU:CD	2.07	0.61
1:A:15:ARG:HB3	1:A:16:PRO:HD3	1.87	0.56
1:B:66:PRO:HB3	1:B:82:VAL:O	2.05	0.56
1:D:72:TYR:OH	1:D:215:HIS:HE1	1.88	0.56
1:B:423:ILE:HA	1:D:516:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:GLN:HE22	1:C:307:ARG:HH11	1.54	0.55
1:C:72:TYR:OH	1:C:215:HIS:HE1	1.90	0.55
1:A:72:TYR:OH	1:A:215:HIS:HE1	1.90	0.54
1:B:72:TYR:OH	1:B:215:HIS:HE1	1.91	0.54
1:C:509:THR:HG23	1:C:511:LYS:H	1.72	0.54
1:D:509:THR:HG23	1:D:511:LYS:H	1.72	0.54
1:B:422:ASP:O	1:D:516:ARG:NH2	2.42	0.53
1:B:70:THR:HG23	1:B:75:LEU:O	2.08	0.52
1:A:60:GLY:HA3	1:A:70:THR:HG21	1.91	0.52
1:C:25:GLN:HG2	1:C:331:GLU:HB2	1.92	0.52
1:D:56:ARG:HD2	1:D:369:GLU:O	2.10	0.51
1:A:394:ASP:OD1	1:A:498:HIS:HD2	1.94	0.51
1:B:25:GLN:HG2	1:B:331:GLU:HB2	1.91	0.51
1:C:222:HIS:HD2	1:C:223:PRO:O	1.93	0.51
1:D:25:GLN:HG2	1:D:331:GLU:HB2	1.93	0.51
1:D:375:ALA:O	1:D:395:GLY:HA3	2.12	0.50
1:B:50:ASP:HB3	1:B:356:ARG:HE	1.75	0.49
1:A:24:ASP:HB3	1:A:222:HIS:HB2	1.94	0.49
1:A:509:THR:HG23	1:A:511:LYS:H	1.77	0.48
1:D:170:HIS:HD2	1:D:187:TYR:OH	1.97	0.48
1:B:508:LEU:HD22	1:D:116:ALA:HB1	1.94	0.48
1:C:394:ASP:OD1	1:C:498:HIS:HD2	1.96	0.48
1:D:50:ASP:HB3	1:D:356:ARG:HE	1.79	0.48
1:C:170:HIS:HD2	1:C:187:TYR:OH	1.98	0.47
1:D:329:HIS:CE1	1:D:341:LYS:HD2	2.50	0.47
1:B:170:HIS:HD2	1:B:187:TYR:OH	1.98	0.47
1:B:222:HIS:HD2	1:B:223:PRO:O	1.98	0.47
1:D:427:GLU:HB2	4:D:2042:HOH:O	2.14	0.47
1:A:170:HIS:HD2	1:A:187:TYR:OH	1.98	0.47
1:A:375:ALA:O	1:A:395:GLY:HA3	2.15	0.47
1:B:394:ASP:OD1	1:B:498:HIS:HD2	1.98	0.46
1:A:50:ASP:HB3	1:A:356:ARG:HE	1.81	0.46
1:C:24:ASP:HB3	1:C:222:HIS:HB2	1.98	0.46
1:B:116:ALA:HB1	1:D:508:LEU:HD22	1.97	0.46
1:A:222:HIS:HD2	1:A:223:PRO:O	1.99	0.45
1:D:304:GLN:O	1:D:307:ARG:HB3	2.16	0.45
1:C:101:ARG:HG2	1:C:107:PRO:HD2	1.98	0.45
1:C:50:ASP:HB3	1:C:356:ARG:HE	1.81	0.45
1:B:427:GLU:HB2	4:B:2068:HOH:O	2.16	0.45
1:D:222:HIS:HD2	1:D:223:PRO:O	2.00	0.45
1:B:20:LEU:O	1:B:215:HIS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ALA:O	1:B:395:GLY:HA3	2.17	0.44
1:C:60:GLY:HA3	1:C:70:THR:HG21	1.99	0.44
1:A:20:LEU:O	1:A:215:HIS:HD2	2.01	0.44
1:D:360:HIS:CE1	1:D:403:GLU:HG2	2.52	0.44
1:B:15:ARG:HB3	1:B:16:PRO:CD	2.47	0.44
1:D:376:ASP:OD2	1:D:411:ARG:NH2	2.51	0.44
1:C:20:LEU:O	1:C:215:HIS:HD2	2.00	0.44
1:B:392:HIS:HE1	1:B:394:ASP:OD1	2.01	0.44
1:C:104:GLY:HA2	1:D:125:ASN:O	2.18	0.43
1:C:219:LEU:O	1:C:222:HIS:HB3	2.18	0.43
1:D:15:ARG:HB3	1:D:16:PRO:HD3	2.00	0.43
1:B:15:ARG:CB	1:B:16:PRO:HD3	2.49	0.43
1:C:302:ASP:HA	1:C:305:LEU:HD12	1.99	0.43
1:D:20:LEU:O	1:D:215:HIS:HD2	2.02	0.43
1:C:392:HIS:HE1	1:C:394:ASP:OD1	2.02	0.42
1:B:24:ASP:HB3	1:B:222:HIS:HB2	2.02	0.42
1:A:116:ALA:HB1	1:C:508:LEU:HD22	2.01	0.42
1:A:331:GLU:HG3	1:A:333:MET:HB2	2.01	0.41
1:B:477:ASP:HB3	1:B:479:ASP:OD1	2.20	0.41
1:D:294:TYR:CG	1:D:333:MET:HE3	2.55	0.41
4:B:2030:HOH:O	1:D:92:ARG:HD2	2.19	0.41
1:A:125:ASN:O	1:B:104:GLY:HA2	2.21	0.41
1:C:294:TYR:CG	1:C:333:MET:HE3	2.55	0.41
1:B:463:ASP:OD1	1:B:465:ALA:HB3	2.20	0.41
1:A:508:LEU:HD22	1:C:116:ALA:HB1	2.03	0.41
4:A:2058:HOH:O	1:C:392:HIS:HD2	2.04	0.41
1:D:477:ASP:HB3	1:D:479:ASP:OD1	2.21	0.41
1:A:294:TYR:CG	1:A:333:MET:HE3	2.56	0.40
1:A:360:HIS:CD2	1:A:403:GLU:HG2	2.57	0.40
1:C:477:ASP:HB3	1:C:479:ASP:OD1	2.21	0.40
1:B:294:TYR:CG	1:B:333:MET:HE3	2.56	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	501/547 (92%)	490 (98%)	11 (2%)	0	100	100
1	B	501/547 (92%)	489 (98%)	12 (2%)	0	100	100
1	C	501/547 (92%)	489 (98%)	12 (2%)	0	100	100
1	D	501/547 (92%)	489 (98%)	11 (2%)	1 (0%)	43	63
All	All	2004/2188 (92%)	1957 (98%)	46 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	231	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/438 (91%)	394 (98%)	6 (2%)	57	80
1	B	400/438 (91%)	396 (99%)	4 (1%)	68	86
1	C	400/438 (91%)	391 (98%)	9 (2%)	44	72
1	D	400/438 (91%)	394 (98%)	6 (2%)	57	80
All	All	1600/1752 (91%)	1575 (98%)	25 (2%)	55	79

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASP
1	A	406	GLU
1	A	444	ILE
1	A	447	GLU
1	A	494	LEU
1	A	517	ARG
1	B	49	GLN

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Mol	Chain	Res	Type
1	B	406	GLU
1	B	411	ARG
1	B	444	ILE
1	C	25	GLN
1	C	50	ASP
1	C	194	THR
1	C	303	THR
1	C	341	LYS
1	C	406	GLU
1	C	444	ILE
1	C	490	LYS
1	C	494	LEU
1	D	50	ASP
1	D	341	LYS
1	D	406	GLU
1	D	444	ILE
1	D	447	GLU
1	D	494	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	170	HIS
1	A	208	GLN
1	A	215	HIS
1	A	391	ASN
1	A	453	HIS
1	A	498	HIS
1	B	161	HIS
1	B	170	HIS
1	B	208	GLN
1	B	215	HIS
1	B	248	ASN
1	B	310	GLN
1	B	391	ASN
1	B	392	HIS
1	B	453	HIS
1	B	498	HIS
1	C	49	GLN
1	C	161	HIS
1	C	170	HIS

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Mol	Chain	Res	Type
1	C	208	GLN
1	C	215	HIS
1	C	304	GLN
1	C	310	GLN
1	C	391	ASN
1	C	392	HIS
1	C	431	HIS
1	C	498	HIS
1	D	77	GLN
1	D	161	HIS
1	D	170	HIS
1	D	208	GLN
1	D	215	HIS
1	D	310	GLN
1	D	360	HIS
1	D	391	ASN
1	D	392	HIS
1	D	431	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](#)

4 non-standard protein/DNA/RNA residues 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
1	DDZ	B	64	1,2	4,6,7	1.58	1 (25%)	3,7,9	1.64	1 (33%)
1	DDZ	D	64	1,2	4,6,7	1.39	1 (25%)	3,7,9	1.80	1 (33%)
1	DDZ	C	64	1,2	4,6,7	1.71	2 (50%)	3,7,9	1.77	1 (33%)
1	DDZ	A	64	1,2	4,6,7	1.42	1 (25%)	3,7,9	1.75	1 (33%)

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
1	DDZ	B	64	1,2	-	0/2/6/8	-
1	DDZ	D	64	1,2	-	0/2/6/8	-
1	DDZ	C	64	1,2	-	0/2/6/8	-
1	DDZ	A	64	1,2	-	0/2/6/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	DDZ	OG1-CB	2.45	1.45	1.40
1	C	64	DDZ	OG2-CB	2.33	1.45	1.40
1	C	64	DDZ	OG1-CB	2.28	1.45	1.40
1	A	64	DDZ	OG2-CB	2.08	1.45	1.40
1	D	64	DDZ	OG2-CB	2.06	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	64	DDZ	O-C-CA	-3.05	116.93	124.77
1	C	64	DDZ	O-C-CA	-2.99	117.07	124.77
1	B	64	DDZ	O-C-CA	-2.81	117.54	124.77
1	A	64	DDZ	O-C-CA	-2.68	117.87	124.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	503/547 (91%)	-0.06	0 100 100	32, 49, 73, 99	0
1	B	503/547 (91%)	0.40	7 (1%) 73 70	38, 60, 84, 115	0
1	C	503/547 (91%)	0.39	21 (4%) 40 36	34, 58, 88, 112	0
1	D	503/547 (91%)	0.79	44 (8%) 16 14	37, 65, 97, 120	0
All	All	2012/2188 (91%)	0.38	72 (3%) 46 41	32, 57, 89, 120	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	340	GLY	4.3
1	D	225	PHE	3.8
1	D	518	PRO	3.7
1	C	518	PRO	3.7
1	D	58	PHE	3.4
1	B	518	PRO	3.3
1	D	40	LYS	3.1
1	D	270	SER	3.1
1	D	180	ILE	3.1
1	D	173	VAL	3.0
1	D	236	THR	3.0
1	D	344	PHE	3.0
1	D	141	ALA	2.8
1	D	169	ILE	2.8
1	D	147	GLU	2.8
1	D	289	ALA	2.8
1	C	40	LYS	2.8
1	D	230	PRO	2.7
1	C	238	SER	2.7
1	C	140	SER	2.7
1	C	189	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	226	SER	2.7
1	D	112	TYR	2.7
1	B	340	GLY	2.6
1	D	272	ILE	2.6
1	D	183	VAL	2.6
1	C	141	ALA	2.6
1	D	331	GLU	2.5
1	D	186	ALA	2.5
1	D	160	GLY	2.5
1	D	242	ALA	2.5
1	B	85	ASN	2.4
1	D	164	ALA	2.4
1	C	176	THR	2.4
1	D	176	THR	2.4
1	C	162	PRO	2.4
1	C	242	ALA	2.4
1	C	37	ALA	2.4
1	D	161	HIS	2.3
1	D	182	ASP	2.3
1	B	465	ALA	2.3
1	C	171	ILE	2.3
1	C	270	SER	2.3
1	B	40	LYS	2.3
1	D	171	ILE	2.2
1	C	282	TRP	2.2
1	D	294	TYR	2.2
1	D	31	LEU	2.2
1	C	15	ARG	2.2
1	C	161	HIS	2.2
1	D	132	TYR	2.2
1	D	298	ILE	2.2
1	D	37	ALA	2.1
1	D	246	ALA	2.1
1	C	295	TYR	2.1
1	D	234	MET	2.1
1	C	132	TYR	2.1
1	D	462	TYR	2.1
1	C	164	ALA	2.1
1	D	189	LYS	2.1
1	D	166	SER	2.1
1	C	177	PRO	2.1
1	D	296	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	63	PRO	2.1
1	D	46	ALA	2.0
1	D	229	GLU	2.0
1	B	511	LYS	2.0
1	C	272	ILE	2.0
1	D	444	ILE	2.0
1	D	237	PRO	2.0
1	C	271	PHE	2.0
1	D	178	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	DDZ	C	64	7/8	0.91	0.10	52,54,61,65	0
1	DDZ	B	64	7/8	0.92	0.08	52,54,56,58	0
1	DDZ	D	64	7/8	0.92	0.09	50,51,58,59	0
1	DDZ	A	64	7/8	0.96	0.07	44,46,52,58	0

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
3	CL	C	1549	1/1	0.85	0.14	98,98,98,98	0
3	CL	D	1549	1/1	0.86	0.23	100,100,100,100	0
3	CL	A	1549	1/1	0.89	0.16	81,81,81,81	0
3	CL	B	1549	1/1	0.92	0.19	85,85,85,85	0
2	MG	B	1001	1/1	0.98	0.05	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	C	1001	1/1	0.99	0.03	35,35,35,35	0
2	MG	D	1001	1/1	0.99	0.05	56,56,56,56	0
2	MG	A	1001	1/1	0.99	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.