



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:54 PM EDT

PDB ID : 3HPH / pdb_00003hph
Title : Closed tetramer of Visna virus integrase (residues 1-219) in complex with LEDGF IBD
Authors : Hare, S.; Wang, J.; Cherepanov, P.
Deposited on : 2009-06-04
Resolution : 2.64 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

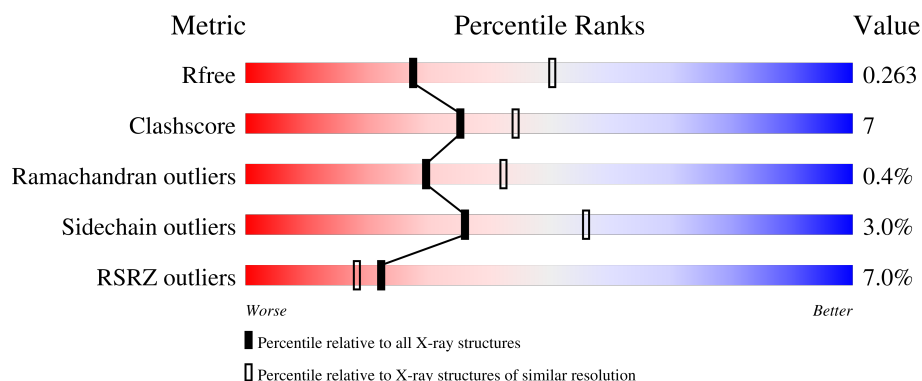
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	219	 4% 79% 10% 11%
1	B	219	 3% 77% 14% 9%
1	C	219	 5% 74% 17% 8%
1	D	219	 5% 75% 14% 11%
2	E	94	 9% 82% 12% 5%

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Mol	Chain	Length	Quality of chain
2	F	94	5% 45% 18% • 36%
2	G	94	11% 40% 16% • 43%
2	H	94	18% 78% 17% • •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8778 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 Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1539	982	259	291	7			
1	B	200	Total	C	N	O	S	0	0	0
			1569	995	271	296	7			
1	C	202	Total	C	N	O	S	0	0	0
			1583	1003	274	299	7			
1	D	196	Total	C	N	O	S	0	0	0
			1554	990	262	295	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P35956
A	2	VAL	-	expression tag	UNP P35956
B	1	MET	-	expression tag	UNP P35956
B	2	VAL	-	expression tag	UNP P35956
C	1	MET	-	expression tag	UNP P35956
C	2	VAL	-	expression tag	UNP P35956
D	1	MET	-	expression tag	UNP P35956
D	2	VAL	-	expression tag	UNP P35956

- Molecule 2 is a protein called PC4 and SFRS1-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	89	Total	C	N	O	S	0	0	0
			730	463	128	132	7			
2	F	60	Total	C	N	O	S	0	0	0
			482	306	87	86	3			
2	G	54	Total	C	N	O	S	0	0	0
			429	272	75	79	3			
2	H	91	Total	C	N	O	S	0	0	0
			739	468	130	134	7			

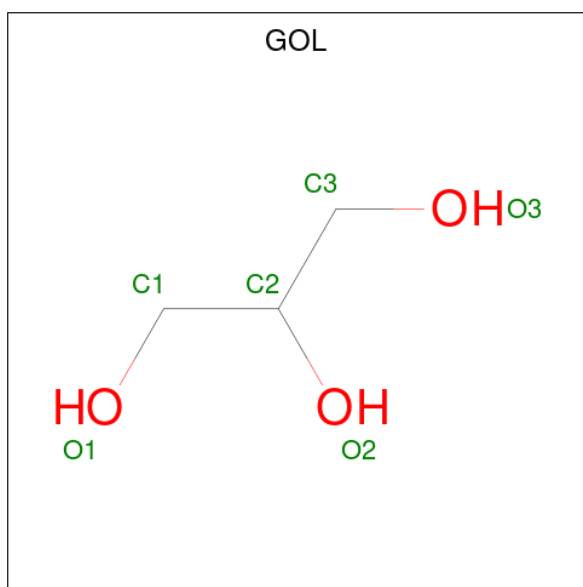
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	436	LEU	-	expression tag	UNP O75475
E	437	GLU	-	expression tag	UNP O75475
E	438	VAL	-	expression tag	UNP O75475
E	439	LEU	-	expression tag	UNP O75475
E	440	PHE	-	expression tag	UNP O75475
E	441	GLN	-	expression tag	UNP O75475
F	436	LEU	-	expression tag	UNP O75475
F	437	GLU	-	expression tag	UNP O75475
F	438	VAL	-	expression tag	UNP O75475
F	439	LEU	-	expression tag	UNP O75475
F	440	PHE	-	expression tag	UNP O75475
F	441	GLN	-	expression tag	UNP O75475
G	436	LEU	-	expression tag	UNP O75475
G	437	GLU	-	expression tag	UNP O75475
G	438	VAL	-	expression tag	UNP O75475
G	439	LEU	-	expression tag	UNP O75475
G	440	PHE	-	expression tag	UNP O75475
G	441	GLN	-	expression tag	UNP O75475
H	436	LEU	-	expression tag	UNP O75475
H	437	GLU	-	expression tag	UNP O75475
H	438	VAL	-	expression tag	UNP O75475
H	439	LEU	-	expression tag	UNP O75475
H	440	PHE	-	expression tag	UNP O75475
H	441	GLN	-	expression tag	UNP O75475

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

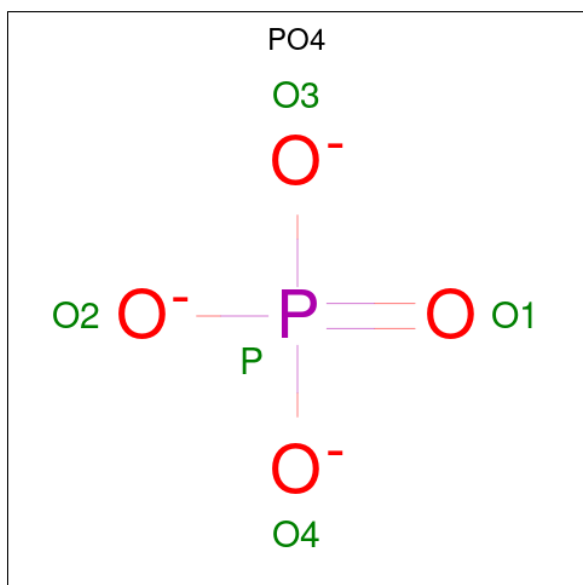
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

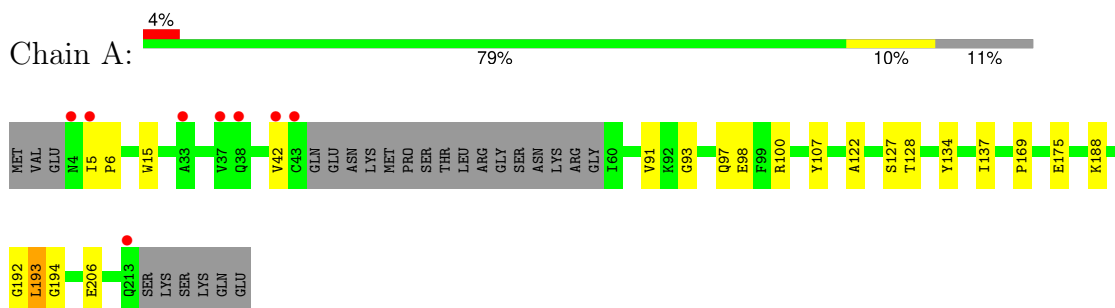
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	28	Total	O	0	0
			28	28		
6	C	34	Total	O	0	0
			34	34		
6	D	14	Total	O	0	0
			14	14		
6	E	6	Total	O	0	0
			6	6		
6	F	1	Total	O	0	0
			1	1		
6	G	2	Total	O	0	0
			2	2		
6	H	7	Total	O	0	0
			7	7		

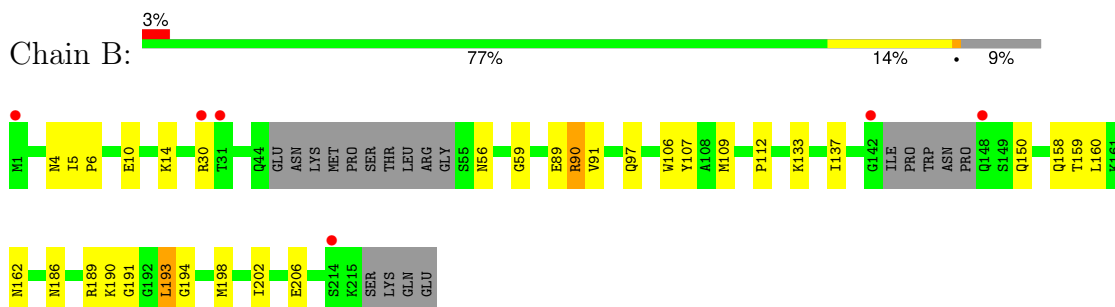
3 Residue-property plots [i](#)

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.

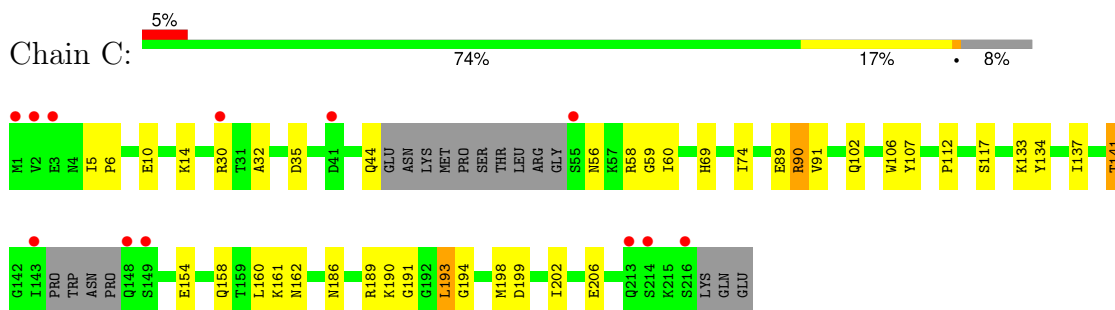
- Molecule 1: Integrase



- Molecule 1: Integrase

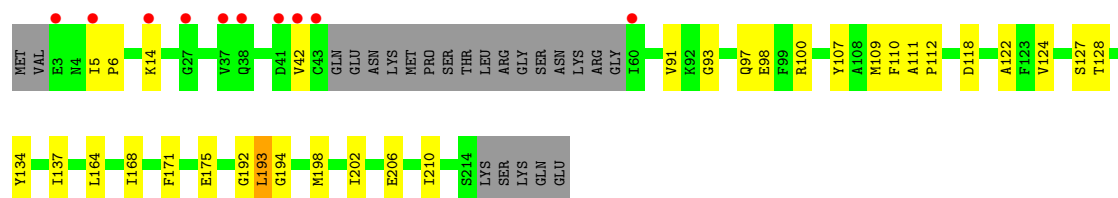


- Molecule 1: Integrase

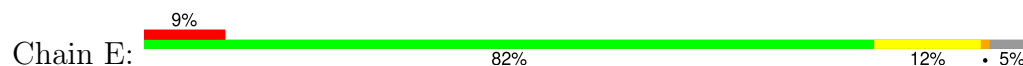


- Molecule 1: Integrase

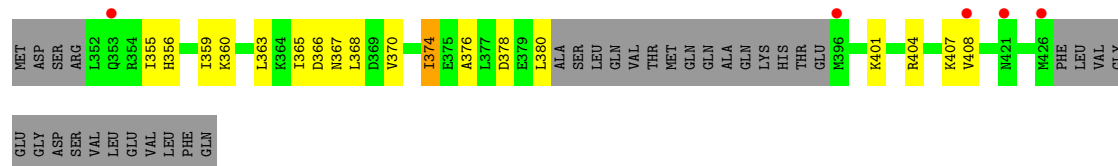
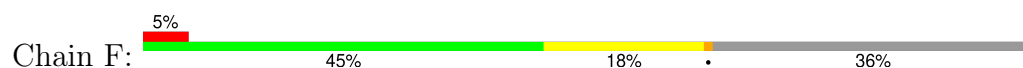




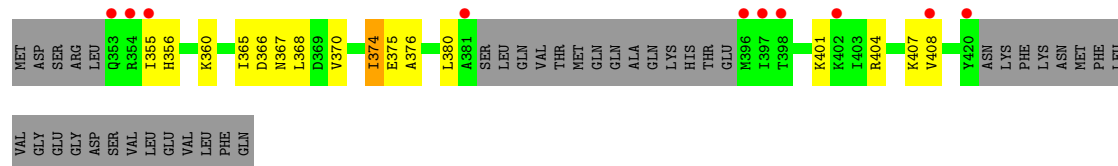
- Molecule 2: PC4 and SFRS1-interacting protein



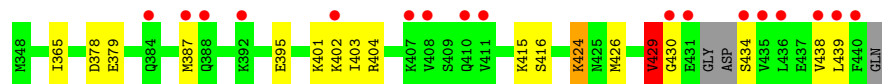
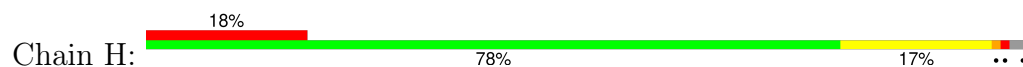
- Molecule 2: PC4 and SFRS1-interacting protein



- Molecule 2: PC4 and SFRS1-interacting protein



- Molecule 2: PC4 and SFRS1-interacting protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.87Å 83.15Å 115.30Å 90.00° 101.96° 90.00°	Depositor
Resolution (Å)	39.01 – 2.64 39.01 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.01-2.64) 99.5 (39.01-2.64)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.253 0.237 , 0.263	Depositor DCC
R_{free} test set	2827 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8778	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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, ZN, GOL

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	0.77	0/1575	0.96	1/2140 (0.0%)
1	B	0.89	0/1600	1.06	8/2166 (0.4%)
1	C	0.89	0/1614	1.08	4/2185 (0.2%)
1	D	0.75	0/1590	0.93	1/2160 (0.0%)
2	E	0.69	0/735	0.94	0/980
2	F	0.58	0/484	0.83	0/644
2	G	0.59	0/430	0.89	0/574
2	H	0.65	0/744	0.93	0/992
All	All	0.78	0/8772	0.98	14/11841 (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	C	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	LEU	N-CA-C	7.13	122.07	113.23
1	C	193	LEU	N-CA-C	6.96	122.63	113.30
1	D	193	LEU	N-CA-C	6.64	121.67	113.50
1	B	186	ASN	CA-C-N	-6.61	115.83	122.77
1	B	186	ASN	C-N-CA	-6.61	115.83	122.77
1	B	109	MET	N-CA-C	6.42	117.93	111.07
1	B	193	LEU	N-CA-C	5.86	121.15	113.30
1	B	159	THR	N-CA-C	-5.44	105.35	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	186	ASN	CA-C-N	-5.41	117.09	122.77
1	C	186	ASN	C-N-CA	-5.41	117.09	122.77
1	B	150	GLN	N-CA-C	5.35	118.33	110.30
1	B	4	ASN	CA-C-N	5.35	124.61	120.33
1	B	4	ASN	C-N-CA	5.35	124.61	120.33
1	C	199	ASP	N-CA-C	-5.24	105.57	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	141	THR	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	1539	0	1476	23	0
1	B	1569	0	1507	19	0
1	C	1583	0	1517	29	0
1	D	1554	0	1489	31	0
2	E	730	0	774	8	0
2	F	482	0	505	12	0
2	G	429	0	452	11	0
2	H	739	0	779	13	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	12	0	16	0	0
4	C	6	0	8	1	0
4	D	6	0	8	0	0
5	B	5	0	0	0	0
5	E	5	0	0	0	0
5	H	5	0	0	1	0
6	A	18	0	0	1	0
6	B	28	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	34	0	0	2	0
6	D	14	0	0	1	0
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	7	0	0	1	0
All	All	8778	0	8531	127	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 7.

All (127) 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)
2:H:387:MET:HE1	2:H:430:GLY:HA2	1.28	1.09
1:C:30:ARG:NH2	1:C:59:GLY:HA2	1.78	0.97
1:D:193:LEU:N	1:D:194:GLY:HA2	1.88	0.89
1:B:30:ARG:NH2	1:B:59:GLY:HA2	1.91	0.85
1:B:90:ARG:HD2	6:B:245:HOH:O	1.76	0.85
1:A:193:LEU:N	1:A:194:GLY:HA2	1.92	0.84
1:C:90:ARG:HD2	6:C:249:HOH:O	1.81	0.81
1:C:30:ARG:HH21	1:C:59:GLY:HA2	1.45	0.80
1:B:30:ARG:HH21	1:B:59:GLY:HA2	1.49	0.77
1:A:97:GLN:HE21	2:F:367:ASN:ND2	1.82	0.76
1:D:5:ILE:HG23	1:D:6:PRO:HD3	1.67	0.75
1:A:100:ARG:HH11	1:A:128:THR:HG22	1.53	0.73
1:D:100:ARG:HH11	1:D:128:THR:HG22	1.54	0.73
1:A:5:ILE:HG23	1:A:6:PRO:HD3	1.73	0.71
1:C:158:GLN:O	1:C:162:ASN:HB2	1.94	0.68
2:H:395:GLU:HB2	6:H:78:HOH:O	1.94	0.68
1:D:97:GLN:HE21	2:G:367:ASN:ND2	1.93	0.67
1:B:97:GLN:HG3	6:E:98:HOH:O	1.95	0.67
1:B:158:GLN:O	1:B:162:ASN:HB2	1.95	0.67
1:A:107:TYR:HD1	1:A:137:ILE:HD11	1.61	0.66
2:E:401:LYS:HA	2:E:404:ARG:HD2	1.78	0.65
1:A:100:ARG:HH11	1:A:128:THR:CG2	2.10	0.64
1:C:191:GLY:O	1:C:194:GLY:HA2	1.99	0.62
1:D:100:ARG:HH11	1:D:128:THR:CG2	2.11	0.62
1:D:107:TYR:CD1	1:D:137:ILE:HD11	2.35	0.62
1:B:193:LEU:N	1:B:194:GLY:HA2	2.15	0.62
2:H:429:VAL:HG12	2:H:429:VAL:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:401:LYS:HA	2:H:404:ARG:HD2	1.82	0.60
1:A:107:TYR:CD1	1:A:137:ILE:HD11	2.36	0.60
1:B:191:GLY:O	1:B:194:GLY:HA2	2.02	0.59
1:D:107:TYR:HD1	1:D:137:ILE:HD11	1.66	0.59
1:C:30:ARG:HH22	1:C:59:GLY:HA2	1.64	0.59
1:A:97:GLN:HE21	2:F:367:ASN:HD21	1.50	0.59
1:D:5:ILE:CG2	1:D:6:PRO:HD3	2.32	0.59
1:C:193:LEU:N	1:C:194:GLY:HA2	2.18	0.57
1:A:91:VAL:HG13	1:A:98:GLU:CD	2.29	0.57
1:A:175:GLU:H	1:A:175:GLU:CD	2.13	0.56
2:H:429:VAL:O	2:H:429:VAL:CG1	2.53	0.56
1:B:189:ARG:O	1:B:190:LYS:HG2	2.04	0.56
1:A:206:GLU:HG2	1:B:206:GLU:HG2	1.87	0.56
1:D:97:GLN:HE21	2:G:367:ASN:HD21	1.53	0.55
1:A:134:TYR:CZ	1:C:14:LYS:HG2	2.42	0.55
1:C:206:GLU:HG2	1:D:206:GLU:HG2	1.88	0.54
1:A:5:ILE:CG2	1:A:6:PRO:HD3	2.37	0.54
1:A:98:GLU:HB3	6:A:224:HOH:O	2.07	0.54
1:C:30:ARG:NH2	1:C:59:GLY:CA	2.63	0.53
1:D:198:MET:O	1:D:202:ILE:HG12	2.08	0.52
1:B:30:ARG:HH21	1:B:59:GLY:CA	2.21	0.52
1:C:107:TYR:CE1	1:C:137:ILE:HD11	2.44	0.52
2:F:356:HIS:CE1	2:F:360:LYS:HE2	2.45	0.52
1:C:106:TRP:CH2	1:C:112:PRO:HG3	2.45	0.52
1:D:193:LEU:HD12	6:D:232:HOH:O	2.09	0.52
1:B:30:ARG:NH2	1:B:59:GLY:CA	2.68	0.51
2:G:356:HIS:CE1	2:G:360:LYS:HE2	2.46	0.51
2:E:403:ILE:HG13	2:E:416:SER:OG	2.10	0.51
2:H:387:MET:CE	2:H:430:GLY:HA2	2.20	0.50
1:B:5:ILE:N	1:B:6:PRO:HD2	2.26	0.50
1:B:106:TRP:CH2	1:B:112:PRO:HG3	2.47	0.50
1:C:5:ILE:N	1:C:6:PRO:HD2	2.26	0.50
1:C:30:ARG:HH21	1:C:60:ILE:H	1.59	0.50
1:D:91:VAL:HG13	1:D:98:GLU:CD	2.36	0.49
1:C:198:MET:HG2	1:C:202:ILE:HD12	1.95	0.49
1:D:134:TYR:CZ	2:G:365:ILE:HG12	2.47	0.49
2:H:401:LYS:O	2:H:404:ARG:HD3	2.12	0.49
1:D:175:GLU:H	1:D:175:GLU:CD	2.21	0.49
1:B:90:ARG:HG3	1:B:91:VAL:N	2.27	0.48
2:E:429:VAL:HG12	2:E:429:VAL:O	2.11	0.48
2:G:355:ILE:HG21	2:G:380:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:SER:OG	2:G:368:LEU:O	2.28	0.48
2:E:401:LYS:O	2:E:404:ARG:HD3	2.13	0.48
1:D:122:ALA:O	1:D:128:THR:HG21	2.13	0.48
1:D:193:LEU:H	1:D:194:GLY:HA2	1.76	0.48
1:C:107:TYR:CD1	1:C:137:ILE:HD11	2.49	0.47
1:C:117:SER:O	1:C:141:THR:HA	2.14	0.47
2:F:355:ILE:HG21	2:F:380:LEU:HD13	1.95	0.47
1:B:189:ARG:C	1:B:190:LYS:HG2	2.40	0.47
1:C:30:ARG:HH21	1:C:59:GLY:CA	2.20	0.47
2:E:429:VAL:O	2:E:429:VAL:CG1	2.62	0.47
1:B:14:LYS:HG2	1:D:134:TYR:CZ	2.49	0.46
1:C:90:ARG:HG3	1:C:91:VAL:N	2.30	0.46
1:D:124:VAL:O	1:D:124:VAL:HG12	2.15	0.46
1:C:198:MET:HE3	4:C:221:GOL:O3	2.16	0.46
1:D:100:ARG:HG3	1:D:128:THR:HG22	1.99	0.45
1:B:107:TYR:CE1	1:B:137:ILE:HD11	2.51	0.45
1:C:102:GLN:NE2	6:C:231:HOH:O	2.50	0.45
1:A:169:PRO:O	2:E:364:LYS:NZ	2.51	0.44
2:G:401:LYS:HA	2:G:404:ARG:HD3	2.00	0.44
2:F:359:ILE:O	2:F:363:LEU:HG	2.18	0.44
2:H:378:ASP:OD1	2:H:415:LYS:NZ	2.48	0.44
2:F:378:ASP:C	2:F:380:LEU:H	2.25	0.44
2:E:387:MET:HE2	2:E:426:MET:O	2.17	0.44
2:H:403:ILE:HG13	2:H:416:SER:OG	2.18	0.43
2:H:434:SER:O	2:H:438:VAL:HG23	2.18	0.43
1:A:91:VAL:HG12	1:A:93:GLY:O	2.18	0.43
1:D:111:ALA:N	1:D:112:PRO:CD	2.81	0.43
1:A:122:ALA:O	1:A:128:THR:HG21	2.18	0.43
2:E:434:SER:O	2:E:438:VAL:HG23	2.19	0.42
1:D:100:ARG:NE	2:G:366:ASP:O	2.44	0.42
2:F:366:ASP:OD1	2:F:366:ASP:N	2.50	0.42
1:A:127:SER:OG	2:F:368:LEU:O	2.36	0.42
1:C:10:GLU:OE2	2:F:407:LYS:HE2	2.18	0.42
1:C:69:HIS:O	1:C:161:LYS:HE2	2.19	0.42
2:H:387:MET:HE2	2:H:426:MET:O	2.19	0.42
1:D:109:MET:HB3	1:D:110:PHE:CD2	2.55	0.42
1:A:15:TRP:CD1	1:A:188:LYS:HE3	2.55	0.42
1:A:175:GLU:CD	1:A:175:GLU:N	2.77	0.42
1:D:171:PHE:CE1	2:H:365:ILE:HB	2.55	0.42
2:F:401:LYS:HA	2:F:404:ARG:HD3	2.01	0.41
1:A:100:ARG:HG3	1:A:128:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:TYR:CZ	2:F:365:ILE:HG12	2.55	0.41
1:D:91:VAL:HG12	1:D:93:GLY:O	2.20	0.41
1:C:32:ALA:O	1:C:35:ASP:HB2	2.20	0.41
2:H:424:LYS:NZ	5:H:2:PO4:O3	2.54	0.41
1:D:118:ASP:OD1	1:D:118:ASP:C	2.64	0.41
2:F:374:ILE:C	2:F:376:ALA:H	2.28	0.41
1:C:69:HIS:CD2	1:C:74:ILE:HG12	2.56	0.41
1:C:58:ARG:HH11	1:C:58:ARG:HD2	1.70	0.41
1:C:189:ARG:C	1:C:190:LYS:HG2	2.46	0.40
2:G:401:LYS:HA	2:G:404:ARG:CD	2.51	0.40
1:A:134:TYR:CE1	1:C:14:LYS:HG2	2.55	0.40
1:B:10:GLU:OE2	2:G:407:LYS:HE2	2.21	0.40
2:G:374:ILE:C	2:G:376:ALA:H	2.29	0.40
1:B:198:MET:HG2	1:B:202:ILE:HD12	2.03	0.40
1:D:109:MET:HB3	1:D:110:PHE:CE2	2.57	0.40
1:C:134:TYR:CZ	1:D:14:LYS:HG2	2.57	0.40
1:D:164:LEU:O	1:D:168:ILE:HG13	2.21	0.40
1:D:210:ILE:O	1:D:210:ILE:CG2	2.69	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	190/219 (87%)	184 (97%)	5 (3%)	1 (0%)	24	36
1	B	194/219 (89%)	188 (97%)	6 (3%)	0	100	100
1	C	196/219 (90%)	190 (97%)	6 (3%)	0	100	100
1	D	192/219 (88%)	186 (97%)	5 (3%)	1 (0%)	24	36
2	E	85/94 (90%)	82 (96%)	3 (4%)	0	100	100
2	F	56/94 (60%)	51 (91%)	5 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	50/94 (53%)	45 (90%)	4 (8%)	1 (2%)	6	8
2	H	87/94 (93%)	80 (92%)	6 (7%)	1 (1%)	11	16
All	All	1050/1252 (84%)	1006 (96%)	40 (4%)	4 (0%)	30	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	GLY
1	D	192	GLY
2	G	375	GLU
2	H	429	VAL

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	163/193 (84%)	162 (99%)	1 (1%)	78	87
1	B	163/193 (84%)	158 (97%)	5 (3%)	35	55
1	C	164/193 (85%)	157 (96%)	7 (4%)	26	42
1	D	165/193 (86%)	164 (99%)	1 (1%)	78	87
2	E	85/88 (97%)	82 (96%)	3 (4%)	32	51
2	F	53/88 (60%)	50 (94%)	3 (6%)	18	31
2	G	48/88 (54%)	45 (94%)	3 (6%)	16	27
2	H	85/88 (97%)	80 (94%)	5 (6%)	18	29
All	All	926/1124 (82%)	898 (97%)	28 (3%)	36	56

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	B	56	ASN
1	B	89	GLU

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Mol	Chain	Res	Type
1	B	90	ARG
1	B	133	LYS
1	B	160	LEU
1	C	44	GLN
1	C	56	ASN
1	C	89	GLU
1	C	90	ARG
1	C	133	LYS
1	C	154	GLU
1	C	160	LEU
1	D	42	VAL
2	E	424	LYS
2	E	429	VAL
2	E	439	LEU
2	F	370	VAL
2	F	374	ILE
2	F	408	VAL
2	G	370	VAL
2	G	374	ILE
2	G	408	VAL
2	H	379	GLU
2	H	402	LYS
2	H	424	LYS
2	H	429	VAL
2	H	439	LEU

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	129	GLN
1	A	162	ASN
1	B	204	ASN
1	C	69	HIS
1	C	102	GLN
1	C	172	ASN
1	C	204	ASN
1	D	129	GLN
1	D	162	ASN
2	E	367	ASN
2	F	361	ASN
2	F	367	ASN

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Mol	Chain	Res	Type
2	G	367	ASN
2	H	367	ASN

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 ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	GOL	D	221	-	5,5,5	0.36	0	5,5,5	0.58	0
5	PO4	E	1	-	4,4,4	0.86	0	6,6,6	0.67	0
4	GOL	A	222	-	5,5,5	0.36	0	5,5,5	0.38	0
5	PO4	B	221	-	4,4,4	0.92	0	6,6,6	0.43	0
4	GOL	C	221	-	5,5,5	0.42	0	5,5,5	0.55	0
5	PO4	H	2	-	4,4,4	0.77	0	6,6,6	0.70	0
4	GOL	A	221	-	5,5,5	0.46	0	5,5,5	0.54	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
4	GOL	A	222	-	-	4/4/4/4	-
4	GOL	D	221	-	-	4/4/4/4	-
4	GOL	C	221	-	-	2/4/4/4	-
4	GOL	A	221	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	222	GOL	O1-C1-C2-C3
4	A	222	GOL	C1-C2-C3-O3
4	C	221	GOL	C1-C2-C3-O3
4	A	222	GOL	O1-C1-C2-O2
4	A	222	GOL	O2-C2-C3-O3
4	D	221	GOL	O1-C1-C2-O2
4	C	221	GOL	O2-C2-C3-O3
4	D	221	GOL	O1-C1-C2-C3
4	D	221	GOL	C1-C2-C3-O3
4	D	221	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	221	GOL	1	0
5	H	2	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 ⓘ

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	194/219 (88%)	0.05	8 (4%)	41	35	6, 21, 45, 53	0
1	B	200/219 (91%)	-0.08	6 (3%)	52	47	3, 13, 47, 55	0
1	C	202/219 (92%)	0.02	12 (5%)	28	23	3, 13, 47, 56	0
1	D	196/219 (89%)	0.08	10 (5%)	33	27	6, 21, 47, 53	0
2	E	89/94 (94%)	0.82	8 (8%)	15	12	12, 38, 89, 98	0
2	F	60/94 (63%)	0.79	5 (8%)	17	13	17, 44, 57, 62	0
2	G	54/94 (57%)	1.11	10 (18%)	3	2	16, 45, 57, 62	0
2	H	91/94 (96%)	0.96	17 (18%)	3	2	12, 38, 89, 98	0
All	All	1086/1252 (86%)	0.26	76 (6%)	22	18	3, 24, 54, 98	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	436	LEU	5.3
2	E	438	VAL	5.2
2	G	353	GLN	5.1
2	H	440	PHE	4.8
2	H	436	LEU	4.6
1	C	143	ILE	4.3
2	H	439	LEU	4.2
2	E	439	LEU	4.2
2	H	438	VAL	4.1
2	E	434	SER	4.1
1	D	38	GLN	4.0
2	E	440	PHE	3.8
1	D	3	GLU	3.8
2	G	355	ILE	3.7
2	H	435	VAL	3.6
1	C	148	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	42	VAL	3.5
2	H	434	SER	3.4
1	B	1	MET	3.4
1	C	55	SER	3.3
1	B	148	GLN	3.2
2	F	421	ASN	3.1
2	G	397	ILE	3.1
2	F	426	MET	3.1
2	G	381	ALA	3.1
2	H	410	GLN	3.1
1	C	149	SER	3.0
2	E	410	GLN	3.0
1	A	5	ILE	3.0
2	G	398	THR	2.9
2	H	388	GLN	2.9
1	C	214	SER	2.9
1	C	1	MET	2.8
1	A	38	GLN	2.8
1	D	42	VAL	2.8
1	C	30	ARG	2.8
2	G	396	MET	2.8
1	B	214	SER	2.6
2	F	396	MET	2.6
2	H	430	GLY	2.6
1	A	37	VAL	2.6
2	G	402	LYS	2.6
1	D	41	ASP	2.6
2	H	407	LYS	2.6
1	A	43	CYS	2.6
2	E	388	GLN	2.6
1	D	43	CYS	2.5
2	H	431	GLU	2.5
1	D	27	GLY	2.5
1	B	30	ARG	2.5
1	C	2	VAL	2.4
1	A	213	GLN	2.4
2	G	354	ARG	2.4
2	H	408	VAL	2.4
2	H	411	VAL	2.4
1	A	33	ALA	2.4
2	H	402	LYS	2.3
1	D	37	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	60	ILE	2.3
2	H	387	MET	2.3
1	C	216	SER	2.3
1	C	41	ASP	2.3
1	D	14	LYS	2.2
2	F	408	VAL	2.2
1	D	5	ILE	2.2
2	G	408	VAL	2.2
2	E	437	GLU	2.2
1	A	4	ASN	2.2
1	C	213	GLN	2.2
1	B	142	GLY	2.2
1	C	3	GLU	2.1
1	B	31	THR	2.1
2	F	353	GLN	2.0
2	G	420	TYR	2.0
2	H	392	LYS	2.0
2	H	384	GLN	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 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
5	PO4	H	2	5/5	0.55	0.20	111,111,111,112	0
5	PO4	E	1	5/5	0.66	0.15	105,105,105,106	0
4	GOL	D	221	6/6	0.77	0.21	87,89,89,89	0
4	GOL	A	222	6/6	0.79	0.21	87,88,88,88	0
5	PO4	B	221	5/5	0.83	0.18	102,103,103,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	221	6/6	0.88	0.20	81,83,84,84	0
4	GOL	C	221	6/6	0.89	0.17	60,61,62,62	0
3	ZN	D	220	1/1	0.96	0.06	34,34,34,34	0
3	ZN	C	220	1/1	0.98	0.03	20,20,20,20	0
3	ZN	A	220	1/1	0.99	0.04	30,30,30,30	0
3	ZN	B	220	1/1	1.00	0.04	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.