



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:11 PM UTC

PDB ID : 8DQN / pdb_00008dqn
Title : Crystal structure of isoaspartyl dipeptidase from *Leucothrix mucor* DSM2157
Authors : Sharon, I.; Schmeing, T.M.
Deposited on : 2022-07-19
Resolution : 1.80 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:

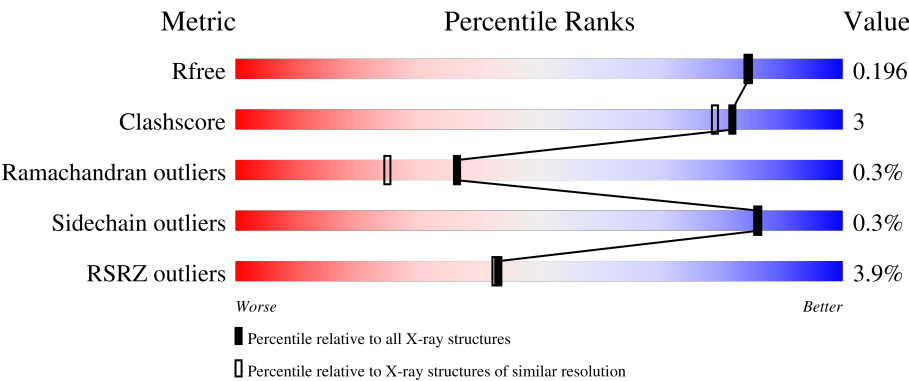
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



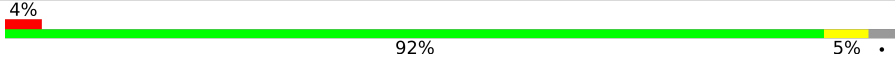
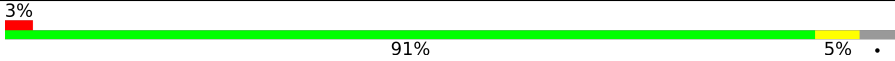
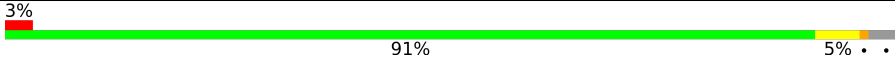
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	394	3% 91%6% ...
1	B	394	3% 90%6% ...
1	C	394	6% 93%5% ...
1	D	394	4% 90%6% ...
1	E	394	4% 91%5% ...

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Mol	Chain	Length	Quality of chain
1	F	394	
1	G	394	
1	H	394	

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
3	ZN	A	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25943 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 Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2856	1809	487	546	14			
1	B	380	Total	C	N	O	S	0	0	0
			2835	1794	484	543	14			
1	C	388	Total	C	N	O	S	0	0	0
			2888	1826	492	556	14			
1	D	380	Total	C	N	O	S	0	0	0
			2837	1796	484	543	14			
1	E	381	Total	C	N	O	S	0	0	0
			2846	1801	485	546	14			
1	F	384	Total	C	N	O	S	0	0	0
			2865	1814	488	549	14			
1	G	379	Total	C	N	O	S	0	0	0
			2826	1787	483	542	14			
1	H	380	Total	C	N	O	S	0	0	0
			2833	1792	484	543	14			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		

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

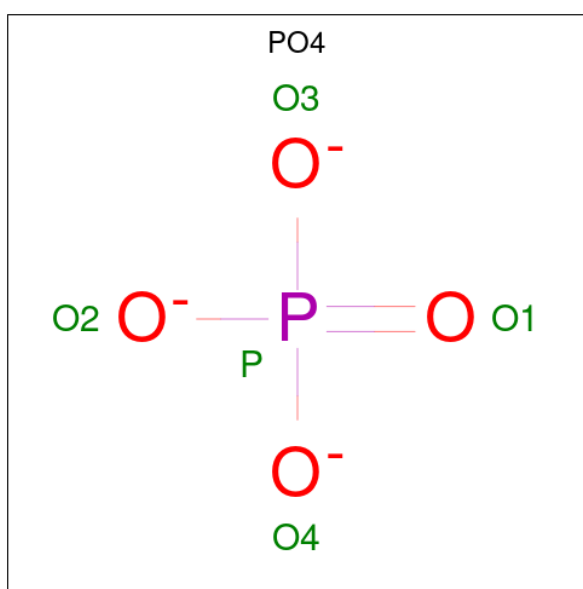
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Zn	0	0
			2	2		
3	B	2	Total	Zn	0	0
			2	2		
3	C	2	Total	Zn	0	0
			2	2		
3	D	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		
3	G	2	Total	Zn	0	0
			2	2		
3	H	2	Total	Zn	0	0
			2	2		

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



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

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

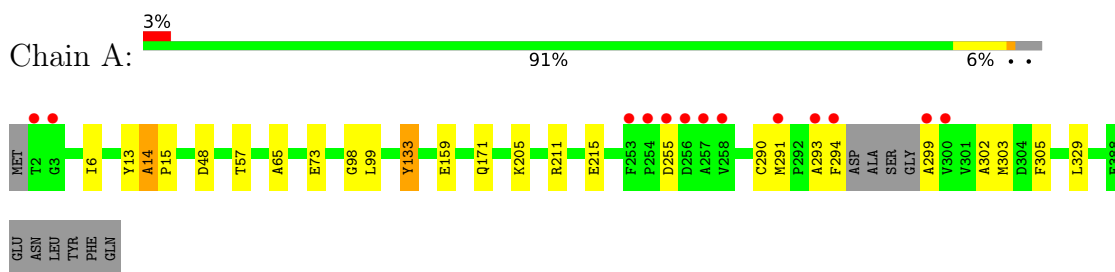
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	385	Total	O	0	0
			385	385		
5	B	389	Total	O	0	0
			389	389		
5	C	367	Total	O	0	0
			367	367		
5	D	400	Total	O	0	0
			400	400		
5	E	353	Total	O	0	0
			353	353		
5	F	371	Total	O	0	0
			371	371		
5	G	393	Total	O	0	0
			393	393		
5	H	395	Total	O	0	0
			395	395		

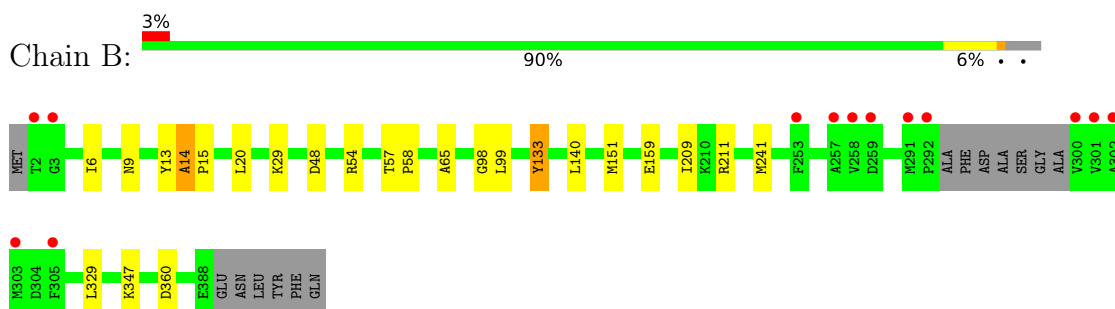
3 Residue-property plots [i](#)

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.

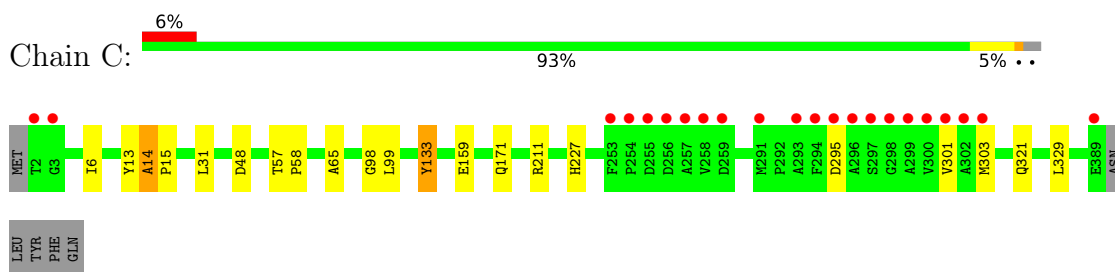
- Molecule 1: Isoaspartyl dipeptidase



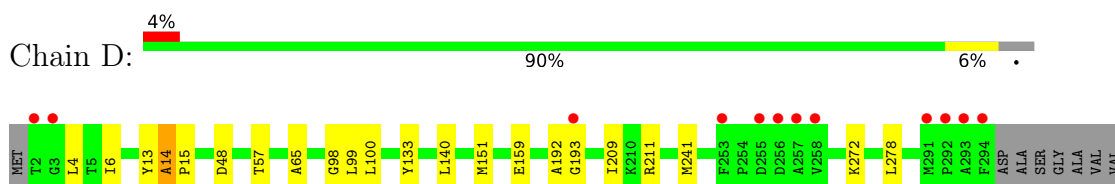
- Molecule 1: Isoaspartyl dipeptidase



- Molecule 1: Isoaspartyl dipeptidase

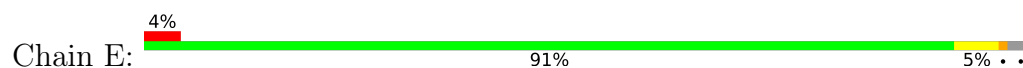


- Molecule 1: Isoaspartyl dipeptidase

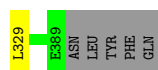




- Molecule 1: Isoaspartyl dipeptidase



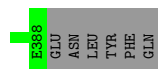
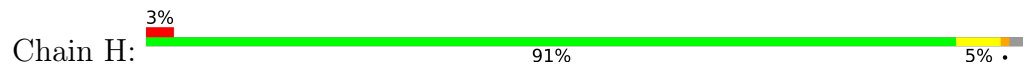
- Molecule 1: Isoaspartyl dipeptidase



- Molecule 1: Isoaspartyl dipeptidase



- Molecule 1: Isoaspartyl dipeptidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.49Å 163.69Å 170.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.34 – 1.80 118.06 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (118.34-1.80) 98.0 (118.06-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.166 , 0.187 0.176 , 0.196	Depositor DCC
R_{free} test set	18699 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25943	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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	1.00	1/2908 (0.0%)	1.21	6/3951 (0.2%)
1	B	0.99	0/2886	1.19	2/3921 (0.1%)
1	C	1.02	0/2941	1.20	2/3997 (0.1%)
1	D	1.02	2/2889 (0.1%)	1.26	7/3924 (0.2%)
1	E	0.99	1/2898 (0.0%)	1.21	3/3936 (0.1%)
1	F	1.00	1/2917 (0.0%)	1.20	3/3963 (0.1%)
1	G	1.00	1/2877 (0.0%)	1.19	2/3908 (0.1%)
1	H	1.01	2/2884 (0.1%)	1.19	5/3918 (0.1%)
All	All	1.01	8/23200 (0.0%)	1.21	30/31518 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	193	GLY	N-CA	6.85	1.55	1.45
1	H	227	HIS	CE1-NE2	5.98	1.38	1.32
1	F	100	LEU	C-O	5.94	1.31	1.23
1	H	100	LEU	C-O	5.69	1.30	1.23
1	G	134	HIS	CE1-NE2	5.25	1.37	1.32
1	E	100	LEU	C-O	5.20	1.30	1.23
1	A	291	MET	CG-SD	5.17	1.93	1.80
1	D	100	LEU	C-O	5.15	1.30	1.23

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	192	ALA	O-C-N	-11.62	107.56	123.01
1	D	192	ALA	CA-C-N	-9.66	102.47	121.41
1	D	192	ALA	C-N-CA	-9.66	102.47	121.41
1	F	305	PHE	CA-C-N	7.49	127.22	120.10
1	F	305	PHE	C-N-CA	7.49	127.22	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	211	ARG	CG-CD-NE	-7.30	95.94	112.00
1	A	305	PHE	CA-C-N	7.20	126.94	120.10
1	A	305	PHE	C-N-CA	7.20	126.94	120.10
1	H	305	PHE	CA-C-N	7.12	126.86	120.10
1	H	305	PHE	C-N-CA	7.12	126.86	120.10
1	D	305	PHE	CA-C-N	7.10	126.85	120.10
1	D	305	PHE	C-N-CA	7.10	126.85	120.10
1	F	211	ARG	CG-CD-NE	-7.10	96.37	112.00
1	E	305	PHE	CA-C-N	6.96	126.72	120.10
1	E	305	PHE	C-N-CA	6.96	126.72	120.10
1	D	211	ARG	CG-CD-NE	-6.92	96.77	112.00
1	C	211	ARG	CG-CD-NE	-6.87	96.90	112.00
1	B	211	ARG	CG-CD-NE	-6.81	97.01	112.00
1	A	211	ARG	CG-CD-NE	-6.56	97.56	112.00
1	G	211	ARG	CG-CD-NE	-6.49	97.73	112.00
1	G	388	GLU	CA-C-O	-6.35	110.01	120.80
1	D	193	GLY	CA-C-O	-5.81	110.47	120.57
1	H	255	ASP	CA-C-N	5.50	127.92	120.38
1	H	255	ASP	C-N-CA	5.50	127.92	120.38
1	B	133	TYR	N-CA-CB	-5.15	102.54	110.42
1	A	133	TYR	N-CA-CB	-5.07	102.66	110.42
1	H	133	TYR	N-CA-CB	-5.07	103.07	110.47
1	C	133	TYR	N-CA-CB	-5.04	102.70	110.42
1	A	255	ASP	CA-C-N	5.04	127.28	120.38
1	A	255	ASP	C-N-CA	5.04	127.28	120.38

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	2856	0	2866	16	0
1	B	2835	0	2847	16	0
1	C	2888	0	2890	17	0
1	D	2837	0	2843	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2846	0	2849	14	0
1	F	2865	0	2872	13	0
1	G	2826	0	2834	13	0
1	H	2833	0	2843	13	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
2	E	6	0	8	1	0
2	F	6	0	8	0	0
2	G	6	0	8	0	0
2	H	6	0	8	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	5	0	0	0	0
5	A	385	0	0	6	0
5	B	389	0	0	4	0
5	C	367	0	0	6	0
5	D	400	0	0	3	1
5	E	353	0	0	3	1
5	F	371	0	0	3	0
5	G	393	0	0	5	1
5	H	395	0	0	4	1
All	All	25943	0	22908	115	2

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 (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:TYR:HE2	5:C:572:HOH:O	1.00	1.31
1:G:133:TYR:HE2	5:G:616:HOH:O	1.17	1.26
1:A:133:TYR:HE2	5:A:559:HOH:O	0.97	1.25
1:H:133:TYR:HE2	5:H:587:HOH:O	1.12	1.23
1:E:133:TYR:HE2	5:E:603:HOH:O	1.19	1.23
1:B:133:TYR:CE2	5:B:510:HOH:O	2.05	1.10
1:B:133:TYR:HE2	5:B:510:HOH:O	1.32	1.08
1:E:133:TYR:CE2	5:E:603:HOH:O	1.96	1.08
1:H:133:TYR:CE2	5:H:587:HOH:O	1.91	1.06
1:C:133:TYR:CE2	5:C:572:HOH:O	1.83	1.01
1:G:133:TYR:CE2	5:G:616:HOH:O	1.97	1.00
1:F:133:TYR:CE2	5:F:512:HOH:O	2.12	0.99
1:A:133:TYR:CE2	5:A:559:HOH:O	1.80	0.99
1:F:133:TYR:HE2	5:F:512:HOH:O	1.47	0.92
1:D:133:TYR:CE2	5:D:504:HOH:O	2.28	0.87
1:F:273:GLU:OE2	5:F:501:HOH:O	2.05	0.75
1:D:133:TYR:HE2	5:D:504:HOH:O	1.68	0.74
1:B:54:ARG:NH1	1:B:360:ASP:OD1	2.21	0.70
1:A:205:LYS:HE3	5:A:776:HOH:O	1.97	0.63
1:B:9:ASN:HA	1:B:20:LEU:HD11	1.81	0.62
1:A:13:TYR:C	1:A:15:PRO:HA	2.31	0.56
1:C:13:TYR:C	1:C:15:PRO:HA	2.31	0.56
1:G:13:TYR:C	1:G:15:PRO:HA	2.31	0.56
1:D:13:TYR:C	1:D:15:PRO:HA	2.31	0.56
1:B:13:TYR:C	1:B:15:PRO:HA	2.31	0.55
1:F:13:TYR:C	1:F:15:PRO:HA	2.32	0.55
1:H:13:TYR:C	1:H:15:PRO:HA	2.32	0.54
1:E:13:TYR:C	1:E:15:PRO:HA	2.32	0.54
1:A:73:GLU:HB3	5:A:503:HOH:O	2.07	0.54
1:C:171:GLN:HG3	5:C:836:HOH:O	2.07	0.54
1:E:373:ARG:HD3	5:E:798:HOH:O	2.10	0.52
1:A:293:ALA:HB3	1:A:302:ALA:HB3	1.92	0.51
1:A:171:GLN:HG3	5:A:856:HOH:O	2.09	0.51
1:E:159:GLU:O	1:E:159:GLU:HG3	2.11	0.51
1:D:159:GLU:HG3	1:D:159:GLU:O	2.11	0.51
1:B:347:LYS:HD3	5:B:663:HOH:O	2.10	0.51
1:H:159:GLU:HG3	1:H:159:GLU:O	2.11	0.51
1:G:2:THR:HG22	5:G:841:HOH:O	2.11	0.50
1:G:159:GLU:O	1:G:159:GLU:HG3	2.11	0.50
1:A:159:GLU:O	1:A:159:GLU:HG3	2.12	0.50
1:F:159:GLU:O	1:F:159:GLU:HG3	2.11	0.50
1:C:159:GLU:O	1:C:159:GLU:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:GLU:O	1:B:159:GLU:HG3	2.12	0.49
1:C:227:HIS:CG	5:C:582:HOH:O	2.65	0.49
1:C:295:ASP:HB3	1:C:301:VAL:HG21	1.93	0.49
2:E:401:GOL:H31	1:F:117:TYR:CD1	2.48	0.49
1:E:209:ILE:HG22	1:E:241:MET:HE1	1.96	0.48
1:A:14:ALA:N	1:A:15:PRO:CA	2.77	0.48
1:C:14:ALA:N	1:C:15:PRO:CA	2.77	0.48
1:D:309:GLU:HG3	5:D:812:HOH:O	2.14	0.47
1:C:14:ALA:N	1:C:15:PRO:HA	2.30	0.47
1:G:14:ALA:N	1:G:15:PRO:CA	2.77	0.47
1:G:227:HIS:CG	5:G:578:HOH:O	2.67	0.47
1:B:14:ALA:N	1:B:15:PRO:CA	2.78	0.47
1:A:14:ALA:N	1:A:15:PRO:HA	2.30	0.47
1:B:14:ALA:N	1:B:15:PRO:HA	2.30	0.47
1:F:14:ALA:N	1:F:15:PRO:CA	2.78	0.47
1:F:14:ALA:N	1:F:15:PRO:HA	2.30	0.46
1:G:14:ALA:N	1:G:15:PRO:HA	2.30	0.46
1:G:73:GLU:OE1	5:G:501:HOH:O	2.20	0.46
1:H:14:ALA:N	1:H:15:PRO:CA	2.79	0.46
1:E:14:ALA:N	1:E:15:PRO:CA	2.78	0.46
1:D:14:ALA:N	1:D:15:PRO:HA	2.31	0.46
1:D:14:ALA:N	1:D:15:PRO:CA	2.78	0.46
1:B:65:ALA:O	1:B:98:GLY:HA2	2.16	0.45
1:F:65:ALA:O	1:F:98:GLY:HA2	2.16	0.45
1:G:65:ALA:O	1:G:98:GLY:HA2	2.17	0.45
1:A:215:GLU:OE1	5:A:501:HOH:O	2.21	0.45
1:E:14:ALA:N	1:E:15:PRO:HA	2.31	0.45
1:H:14:ALA:N	1:H:15:PRO:HA	2.32	0.45
1:A:65:ALA:O	1:A:98:GLY:HA2	2.17	0.45
1:G:209:ILE:HG22	1:G:241:MET:HE1	1.98	0.45
1:H:57:THR:HB	1:H:329:LEU:HD21	1.99	0.45
1:F:140:LEU:HD23	1:F:151:MET:HE3	1.99	0.45
1:H:140:LEU:HD23	1:H:151:MET:HE3	1.99	0.44
1:H:209:ILE:HG22	1:H:241:MET:HE1	1.98	0.44
1:E:65:ALA:O	1:E:98:GLY:HA2	2.17	0.44
1:C:65:ALA:O	1:C:98:GLY:HA2	2.18	0.44
1:G:57:THR:HB	1:G:329:LEU:HD21	1.99	0.44
1:A:6:ILE:HG23	1:A:48:ASP:HA	2.00	0.44
1:H:65:ALA:O	1:H:98:GLY:HA2	2.17	0.44
1:C:57:THR:HB	1:C:329:LEU:HD21	2.00	0.43
1:B:57:THR:HB	1:B:329:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:HG23	1:D:48:ASP:HA	2.00	0.43
1:H:2:THR:HG22	5:H:723:HOH:O	2.17	0.43
1:C:321:GLN:HG3	5:C:752:HOH:O	2.18	0.43
1:B:29:LYS:HE3	5:B:624:HOH:O	2.19	0.43
1:E:57:THR:HB	1:E:329:LEU:HD21	2.00	0.43
1:F:57:THR:HB	1:F:329:LEU:HD21	2.01	0.43
1:D:65:ALA:O	1:D:98:GLY:HA2	2.18	0.43
1:D:209:ILE:HG22	1:D:241:MET:HE1	2.00	0.43
1:B:6:ILE:HG23	1:B:48:ASP:HA	2.00	0.43
1:D:140:LEU:HD23	1:D:151:MET:HE3	2.01	0.43
1:A:57:THR:HB	1:A:329:LEU:HD21	2.01	0.43
1:C:6:ILE:HG23	1:C:48:ASP:HA	2.01	0.43
1:E:6:ILE:HG23	1:E:48:ASP:HA	2.01	0.43
1:D:57:THR:HB	1:D:329:LEU:HD21	2.01	0.42
1:B:140:LEU:HD23	1:B:151:MET:HE3	2.01	0.42
1:E:13:TYR:O	1:E:58:PRO:HD3	2.20	0.42
1:C:31:LEU:HD13	1:D:4:LEU:HD21	2.02	0.42
1:E:140:LEU:HD23	1:E:151:MET:HE3	2.01	0.42
1:G:6:ILE:HG23	1:G:48:ASP:HA	2.01	0.42
1:C:321:GLN:CG	5:C:752:HOH:O	2.66	0.42
1:F:209:ILE:HG22	1:F:241:MET:HE1	2.02	0.41
1:H:6:ILE:HG23	1:H:48:ASP:HA	2.02	0.41
1:A:294:PHE:HA	1:A:299:ALA:O	2.20	0.41
1:E:211:ARG:HG3	1:E:215:GLU:OE2	2.21	0.41
1:C:13:TYR:O	1:C:58:PRO:HD3	2.21	0.40
1:F:151:MET:HG3	1:F:154:ILE:HD12	2.03	0.40
1:A:290:CYS:SG	1:A:303:MET:SD	3.19	0.40
1:B:13:TYR:O	1:B:58:PRO:HD3	2.22	0.40
1:B:209:ILE:HG22	1:B:241:MET:HE1	2.02	0.40
1:H:29:LYS:HE2	5:H:653:HOH:O	2.21	0.40
1:C:303:MET:HE2	1:C:303:MET:HB2	1.94	0.40
1:D:272:LYS:HD3	1:D:278:LEU:HD11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:506:HOH:O	5:G:733:HOH:O[4_445]	2.11	0.09
5:E:709:HOH:O	5:H:693:HOH:O[4_545]	2.18	0.02

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	379/394 (96%)	368 (97%)	10 (3%)	1 (0%)	36	25
1	B	376/394 (95%)	367 (98%)	8 (2%)	1 (0%)	36	25
1	C	386/394 (98%)	375 (97%)	10 (3%)	1 (0%)	36	25
1	D	376/394 (95%)	364 (97%)	11 (3%)	1 (0%)	36	25
1	E	377/394 (96%)	366 (97%)	10 (3%)	1 (0%)	36	25
1	F	380/394 (96%)	370 (97%)	9 (2%)	1 (0%)	36	25
1	G	375/394 (95%)	365 (97%)	9 (2%)	1 (0%)	36	25
1	H	376/394 (95%)	365 (97%)	10 (3%)	1 (0%)	36	25
All	All	3025/3152 (96%)	2940 (97%)	77 (2%)	8 (0%)	36	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	ALA
1	A	14	ALA
1	C	14	ALA
1	D	14	ALA
1	E	14	ALA
1	F	14	ALA
1	G	14	ALA
1	H	14	ALA

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	299/308 (97%)	298 (100%)	1 (0%)	86	86
1	B	298/308 (97%)	297 (100%)	1 (0%)	86	86
1	C	302/308 (98%)	301 (100%)	1 (0%)	86	86
1	D	297/308 (96%)	296 (100%)	1 (0%)	86	86
1	E	298/308 (97%)	297 (100%)	1 (0%)	86	86
1	F	300/308 (97%)	299 (100%)	1 (0%)	86	86
1	G	296/308 (96%)	295 (100%)	1 (0%)	86	86
1	H	297/308 (96%)	296 (100%)	1 (0%)	86	86
All	All	2387/2464 (97%)	2379 (100%)	8 (0%)	86	86

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	B	99	LEU
1	C	99	LEU
1	D	99	LEU
1	E	99	LEU
1	F	99	LEU
1	G	99	LEU
1	H	99	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	280	GLN
1	B	16	GLN
1	B	280	GLN
1	B	338	HIS
1	C	16	GLN
1	C	280	GLN
1	C	338	HIS
1	D	16	GLN
1	D	224	ASN
1	D	280	GLN
1	D	338	HIS
1	E	16	GLN
1	E	87	GLN

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Mol	Chain	Res	Type
1	E	280	GLN
1	E	338	HIS
1	F	16	GLN
1	F	280	GLN
1	F	338	HIS
1	G	16	GLN
1	G	280	GLN
1	G	338	HIS
1	H	16	GLN
1	H	280	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 16 are monoatomic - leaving 16 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	$\# Z > 2$
2	GOL	B	401	-	5,5,5	0.24	0	5,5,5	0.64	0
2	GOL	G	401	-	5,5,5	0.18	0	5,5,5	0.31	0
4	PO4	E	404	-	4,4,4	0.24	0	6,6,6	0.70	0
4	PO4	G	404	-	4,4,4	1.15	1 (25%)	6,6,6	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	401	-	5,5,5	0.05	0	5,5,5	0.36	0
2	GOL	E	401	-	5,5,5	0.23	0	5,5,5	1.00	0
2	GOL	H	401	-	5,5,5	0.17	0	5,5,5	0.48	0
4	PO4	D	404	-	4,4,4	1.02	0	6,6,6	0.66	0
2	GOL	D	401	-	5,5,5	0.12	0	5,5,5	0.21	0
2	GOL	C	401	-	5,5,5	0.18	0	5,5,5	0.84	0
2	GOL	F	401	-	5,5,5	0.19	0	5,5,5	0.60	0
4	PO4	A	404	-	4,4,4	1.24	1 (25%)	6,6,6	0.48	0
4	PO4	F	404	-	4,4,4	1.07	0	6,6,6	0.71	0
4	PO4	H	404	-	4,4,4	0.88	0	6,6,6	0.43	0
4	PO4	C	404	-	4,4,4	0.95	0	6,6,6	0.51	0
4	PO4	B	404	-	4,4,4	0.90	0	6,6,6	0.59	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	GOL	B	401	-	-	0/4/4/4	-
2	GOL	G	401	-	-	2/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-
2	GOL	E	401	-	-	2/4/4/4	-
2	GOL	H	401	-	-	2/4/4/4	-
2	GOL	D	401	-	-	2/4/4/4	-
2	GOL	C	401	-	-	0/4/4/4	-
2	GOL	F	401	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	PO4	P-O1	2.17	1.55	1.50
4	G	404	PO4	P-O1	2.03	1.55	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	E	401	GOL	C1-C2-C3-O3
2	F	401	GOL	O1-C1-C2-C3
2	G	401	GOL	O1-C1-C2-C3
2	H	401	GOL	O1-C1-C2-O2
2	H	401	GOL	O1-C1-C2-C3
2	D	401	GOL	O1-C1-C2-O2
2	E	401	GOL	O2-C2-C3-O3
2	G	401	GOL	O1-C1-C2-O2
2	F	401	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	GOL	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	383/394 (97%)	-0.13	13 (3%)	48	48	19, 27, 50, 114	0
1	B	380/394 (96%)	-0.20	13 (3%)	48	48	19, 27, 58, 111	0
1	C	388/394 (98%)	-0.09	22 (5%)	29	28	18, 26, 67, 98	0
1	D	380/394 (96%)	-0.20	15 (3%)	43	43	18, 26, 55, 116	0
1	E	381/394 (96%)	0.01	15 (3%)	43	43	18, 29, 59, 117	0
1	F	384/394 (97%)	-0.11	17 (4%)	39	38	19, 27, 64, 130	0
1	G	379/394 (96%)	-0.27	10 (2%)	57	57	18, 26, 52, 94	0
1	H	380/394 (96%)	-0.20	13 (3%)	48	48	18, 26, 55, 98	0
All	All	3055/3152 (96%)	-0.15	118 (3%)	43	43	18, 27, 59, 130	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	299	ALA	6.4
1	C	2	THR	6.4
1	C	293	ALA	6.3
1	G	2	THR	6.2
1	E	294	PHE	6.1
1	C	300	VAL	6.0
1	H	293	ALA	5.9
1	C	296	ALA	5.9
1	A	257	ALA	5.7
1	A	294	PHE	5.5
1	E	2	THR	5.5
1	H	2	THR	5.5
1	C	257	ALA	5.4
1	A	253	PHE	5.2
1	D	294	PHE	5.2
1	H	301	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	291	MET	5.2
1	H	291	MET	5.1
1	F	294	PHE	5.0
1	B	300	VAL	5.0
1	F	300	VAL	5.0
1	C	301	VAL	4.9
1	D	291	MET	4.9
1	B	301	VAL	4.8
1	C	253	PHE	4.8
1	A	300	VAL	4.7
1	F	302	ALA	4.7
1	C	295	ASP	4.6
1	F	293	ALA	4.6
1	C	258	VAL	4.6
1	D	258	VAL	4.5
1	B	302	ALA	4.5
1	E	302	ALA	4.4
1	F	299	ALA	4.4
1	D	2	THR	4.3
1	G	293	ALA	4.3
1	H	258	VAL	4.2
1	D	257	ALA	4.2
1	B	2	THR	4.2
1	H	305	PHE	4.2
1	G	302	ALA	4.2
1	B	291	MET	4.2
1	D	302	ALA	4.2
1	B	305	PHE	4.1
1	G	292	PRO	4.1
1	F	2	THR	4.1
1	C	294	PHE	4.1
1	A	258	VAL	4.1
1	C	297	SER	4.1
1	D	305	PHE	4.1
1	D	292	PRO	4.0
1	A	291	MET	4.0
1	C	298	GLY	3.9
1	C	302	ALA	3.9
1	E	258	VAL	3.9
1	C	299	ALA	3.8
1	F	291	MET	3.7
1	B	258	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	253	PHE	3.7
1	A	256	ASP	3.7
1	G	3	GLY	3.7
1	A	293	ALA	3.6
1	A	255	ASP	3.6
1	A	254	PRO	3.6
1	B	292	PRO	3.6
1	E	292	PRO	3.6
1	A	2	THR	3.6
1	B	253	PHE	3.6
1	D	253	PHE	3.6
1	D	293	ALA	3.5
1	C	3	GLY	3.5
1	F	301	VAL	3.4
1	E	305	PHE	3.4
1	F	305	PHE	3.3
1	H	257	ALA	3.2
1	H	3	GLY	3.2
1	E	293	ALA	3.2
1	D	3	GLY	3.1
1	G	304	ASP	3.1
1	E	303	MET	3.1
1	H	292	PRO	3.0
1	B	257	ALA	3.0
1	E	304	ASP	2.9
1	G	291	MET	2.9
1	G	303	MET	2.8
1	F	3	GLY	2.8
1	B	303	MET	2.8
1	C	255	ASP	2.7
1	E	257	ALA	2.7
1	F	253	PHE	2.7
1	E	307	ARG	2.7
1	D	256	ASP	2.6
1	F	257	ALA	2.6
1	G	305	PHE	2.6
1	H	253	PHE	2.6
1	B	259	ASP	2.6
1	C	259	ASP	2.6
1	H	302	ALA	2.6
1	C	291	MET	2.5
1	E	256	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	2.5
1	E	3	GLY	2.5
1	F	303	MET	2.4
1	H	304	ASP	2.4
1	F	258	VAL	2.4
1	D	255	ASP	2.3
1	C	303	MET	2.3
1	B	3	GLY	2.3
1	D	303	MET	2.3
1	F	292	PRO	2.3
1	D	193	GLY	2.3
1	C	254	PRO	2.2
1	H	303	MET	2.2
1	G	258	VAL	2.2
1	A	3	GLY	2.2
1	F	254	PRO	2.1
1	C	389	GLU	2.1
1	F	307	ARG	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
3	ZN	G	403	1/1	0.72	0.33	100,100,100,100	0
3	ZN	D	403	1/1	0.77	0.34	96,96,96,96	0
3	ZN	A	403	1/1	0.78	0.51	101,101,101,101	0
3	ZN	C	403	1/1	0.78	0.34	109,109,109,109	0
3	ZN	B	403	1/1	0.79	0.35	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	H	403	1/1	0.79	0.37	113,113,113,113	0
3	ZN	E	403	1/1	0.83	0.38	92,92,92,92	0
3	ZN	F	403	1/1	0.85	0.34	95,95,95,95	0
4	PO4	C	404	5/5	0.86	0.18	68,89,95,97	0
4	PO4	H	404	5/5	0.86	0.14	53,53,68,75	0
4	PO4	E	404	5/5	0.89	0.15	61,74,85,92	0
4	PO4	G	404	5/5	0.90	0.13	56,66,73,78	0
3	ZN	E	402	1/1	0.90	0.26	87,87,87,87	0
4	PO4	A	404	5/5	0.91	0.11	43,45,61,66	0
4	PO4	B	404	5/5	0.91	0.12	57,66,81,83	0
4	PO4	D	404	5/5	0.92	0.11	53,56,67,68	0
4	PO4	F	404	5/5	0.92	0.11	57,65,69,69	0
2	GOL	C	401	6/6	0.93	0.10	28,33,36,40	0
3	ZN	G	402	1/1	0.94	0.20	76,76,76,76	0
2	GOL	F	401	6/6	0.94	0.11	28,34,41,41	0
3	ZN	H	402	1/1	0.94	0.29	78,78,78,78	0
2	GOL	B	401	6/6	0.95	0.09	29,33,37,38	0
3	ZN	D	402	1/1	0.95	0.25	76,76,76,76	0
2	GOL	A	401	6/6	0.95	0.09	27,32,34,44	0
3	ZN	B	402	1/1	0.95	0.26	83,83,83,83	0
2	GOL	E	401	6/6	0.95	0.10	26,36,38,46	0
3	ZN	C	402	1/1	0.95	0.18	75,75,75,75	0
2	GOL	H	401	6/6	0.96	0.07	28,30,33,37	0
3	ZN	A	402	1/1	0.96	0.23	76,76,76,76	0
3	ZN	F	402	1/1	0.96	0.24	73,73,73,73	0
2	GOL	D	401	6/6	0.96	0.08	27,33,34,43	0
2	GOL	G	401	6/6	0.97	0.07	27,28,31,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.