



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:33 PM UTC

PDB ID : 9YWI / pdb_00009ywi
Title : Crystal structure of a Glyceraldehyde-3-phosphate dehydrogenase from Bordetella pertussis (monoclinic P form)
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2025-10-24
Resolution : 2.00 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

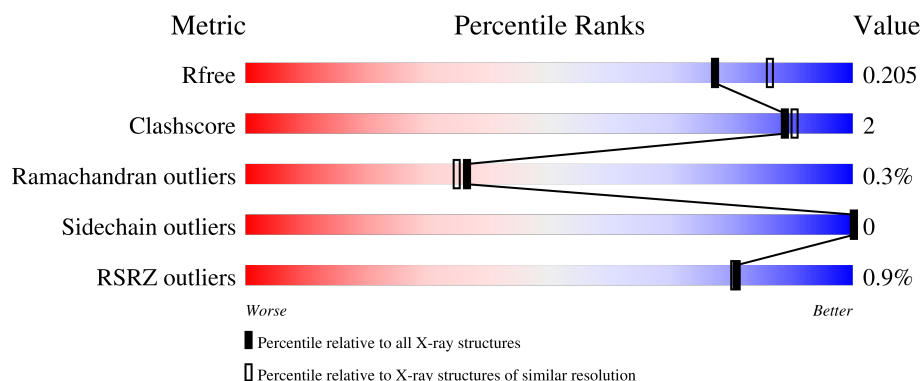
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	344	93% 5%
1	B	344	91% 7%
1	C	344	92% 6%
1	D	344	92% 6%
1	E	344	95% 2%

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Mol	Chain	Length	Quality of chain
1	F	344	94% ..
1	G	344	94% ..
1	H	344	95% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22450 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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2549	1603	445	492	9			
1	B	336	Total	C	N	O	S	0	3	0
			2558	1610	445	493	10			
1	C	336	Total	C	N	O	S	0	3	0
			2550	1603	445	492	10			
1	D	336	Total	C	N	O	S	0	1	0
			2533	1593	443	488	9			
1	E	343	Total	C	N	O	S	0	2	0
			2594	1632	456	495	11			
1	F	336	Total	C	N	O	S	0	2	0
			2549	1603	447	490	9			
1	G	336	Total	C	N	O	S	0	1	0
			2537	1596	444	488	9			
1	H	338	Total	C	N	O	S	0	1	0
			2562	1612	451	489	10			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP Q7VZB9
A	-6	ALA	-	expression tag	UNP Q7VZB9
A	-5	HIS	-	expression tag	UNP Q7VZB9
A	-4	HIS	-	expression tag	UNP Q7VZB9
A	-3	HIS	-	expression tag	UNP Q7VZB9
A	-2	HIS	-	expression tag	UNP Q7VZB9
A	-1	HIS	-	expression tag	UNP Q7VZB9
A	0	HIS	-	expression tag	UNP Q7VZB9
B	-7	MET	-	expression tag	UNP Q7VZB9
B	-6	ALA	-	expression tag	UNP Q7VZB9
B	-5	HIS	-	expression tag	UNP Q7VZB9
B	-4	HIS	-	expression tag	UNP Q7VZB9
B	-3	HIS	-	expression tag	UNP Q7VZB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q7VZB9
B	-1	HIS	-	expression tag	UNP Q7VZB9
B	0	HIS	-	expression tag	UNP Q7VZB9
C	-7	MET	-	expression tag	UNP Q7VZB9
C	-6	ALA	-	expression tag	UNP Q7VZB9
C	-5	HIS	-	expression tag	UNP Q7VZB9
C	-4	HIS	-	expression tag	UNP Q7VZB9
C	-3	HIS	-	expression tag	UNP Q7VZB9
C	-2	HIS	-	expression tag	UNP Q7VZB9
C	-1	HIS	-	expression tag	UNP Q7VZB9
C	0	HIS	-	expression tag	UNP Q7VZB9
D	-7	MET	-	expression tag	UNP Q7VZB9
D	-6	ALA	-	expression tag	UNP Q7VZB9
D	-5	HIS	-	expression tag	UNP Q7VZB9
D	-4	HIS	-	expression tag	UNP Q7VZB9
D	-3	HIS	-	expression tag	UNP Q7VZB9
D	-2	HIS	-	expression tag	UNP Q7VZB9
D	-1	HIS	-	expression tag	UNP Q7VZB9
D	0	HIS	-	expression tag	UNP Q7VZB9
E	-7	MET	-	expression tag	UNP Q7VZB9
E	-6	ALA	-	expression tag	UNP Q7VZB9
E	-5	HIS	-	expression tag	UNP Q7VZB9
E	-4	HIS	-	expression tag	UNP Q7VZB9
E	-3	HIS	-	expression tag	UNP Q7VZB9
E	-2	HIS	-	expression tag	UNP Q7VZB9
E	-1	HIS	-	expression tag	UNP Q7VZB9
E	0	HIS	-	expression tag	UNP Q7VZB9
F	-7	MET	-	expression tag	UNP Q7VZB9
F	-6	ALA	-	expression tag	UNP Q7VZB9
F	-5	HIS	-	expression tag	UNP Q7VZB9
F	-4	HIS	-	expression tag	UNP Q7VZB9
F	-3	HIS	-	expression tag	UNP Q7VZB9
F	-2	HIS	-	expression tag	UNP Q7VZB9
F	-1	HIS	-	expression tag	UNP Q7VZB9
F	0	HIS	-	expression tag	UNP Q7VZB9
G	-7	MET	-	expression tag	UNP Q7VZB9
G	-6	ALA	-	expression tag	UNP Q7VZB9
G	-5	HIS	-	expression tag	UNP Q7VZB9
G	-4	HIS	-	expression tag	UNP Q7VZB9
G	-3	HIS	-	expression tag	UNP Q7VZB9
G	-2	HIS	-	expression tag	UNP Q7VZB9
G	-1	HIS	-	expression tag	UNP Q7VZB9

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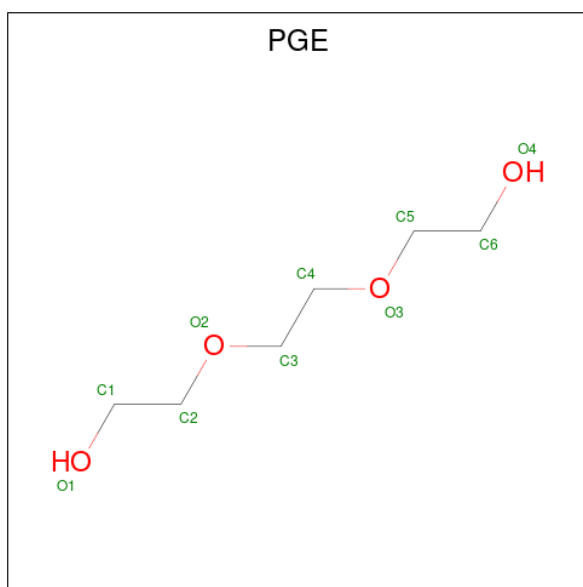
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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q7VZB9
H	-7	MET	-	expression tag	UNP Q7VZB9
H	-6	ALA	-	expression tag	UNP Q7VZB9
H	-5	HIS	-	expression tag	UNP Q7VZB9
H	-4	HIS	-	expression tag	UNP Q7VZB9
H	-3	HIS	-	expression tag	UNP Q7VZB9
H	-2	HIS	-	expression tag	UNP Q7VZB9
H	-1	HIS	-	expression tag	UNP Q7VZB9
H	0	HIS	-	expression tag	UNP Q7VZB9

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

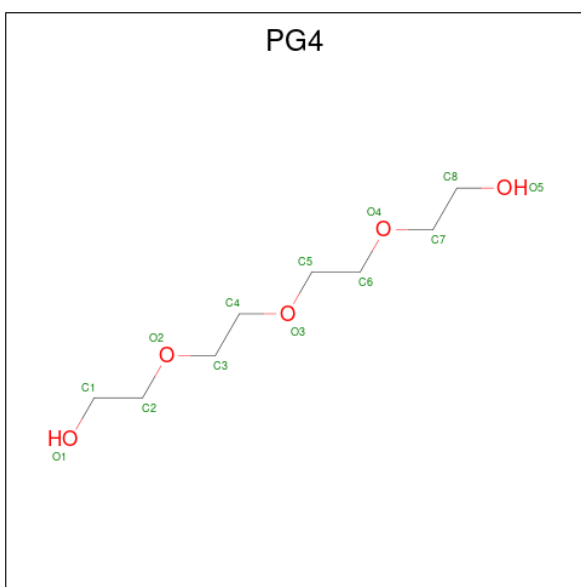
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	3	Total Mg 3 3	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



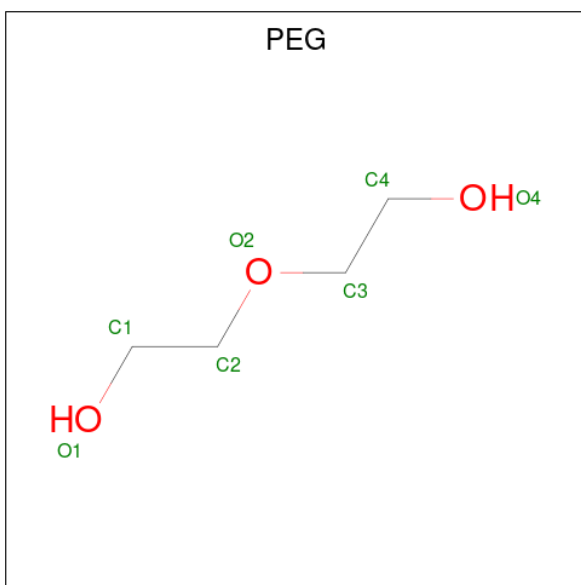
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



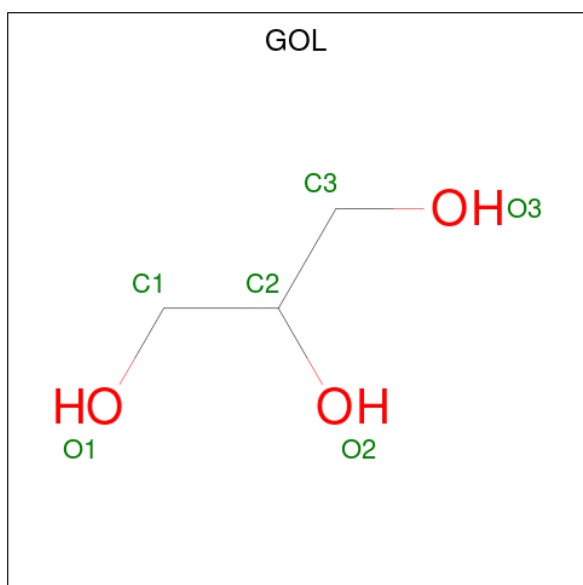
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	B	1	Total	C	O	0	0
			13	8	5		
4	G	1	Total	C	O	0	0
			13	8	5		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	E	1	Total C O 7 4 3	0	0
5	F	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	G	1	Total C O 7 4 3	0	0
5	H	1	Total C O 7 4 3	0	0

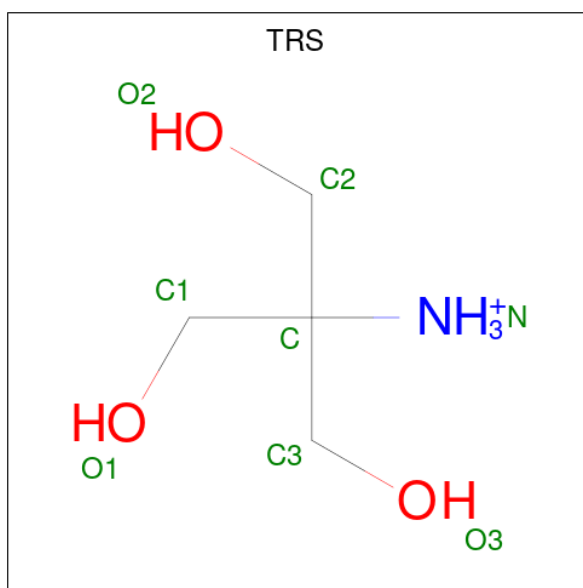
- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS)

(formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	263	Total	O	0	0
			263	263		
8	B	236	Total	O	0	0
			236	236		
8	C	176	Total	O	0	0
			176	176		
8	D	148	Total	O	0	0
			148	148		
8	E	280	Total	O	0	0
			280	280		
8	F	243	Total	O	0	0
			243	243		
8	G	221	Total	O	0	0
			221	221		
8	H	213	Total	O	0	0
			213	213		

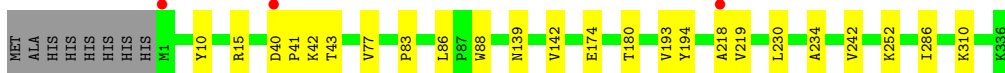
3 Residue-property plots [i](#)

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: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.47Å 122.98Å 150.57Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	49.08 – 2.00 49.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.08-2.00) 99.9 (49.08-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.00Å)	Xtriage
Refinement program	PHENIX (2.0_5855: ???)	Depositor
R, R_{free}	0.169 , 0.203 0.175 , 0.205	Depositor DCC
R_{free} test set	10020 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.088 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22450	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, PG4, MG, TRS, PEG

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	0.18	0/2596	0.36	0/3529
1	B	0.18	0/2611	0.37	0/3549
1	C	0.14	0/2603	0.32	0/3541
1	D	0.17	0/2580	0.36	0/3511
1	E	0.15	0/2648	0.35	0/3602
1	F	0.17	0/2599	0.35	0/3534
1	G	0.16	0/2584	0.34	0/3515
1	H	0.15	0/2610	0.32	0/3547
All	All	0.16	0/20831	0.35	0/28328

There are no bond length outliers.

There are no bond angle outliers.

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	2549	0	2562	10	0
1	B	2558	0	2578	14	0
1	C	2550	0	2551	13	0
1	D	2533	0	2532	12	0
1	E	2594	0	2585	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2549	0	2560	8	0
1	G	2537	0	2543	12	0
1	H	2562	0	2577	9	0
2	A	1	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	10	0	14	0	0
3	B	20	0	28	0	0
3	C	10	0	14	1	0
3	D	10	0	14	0	0
3	E	10	0	14	0	0
3	F	10	0	14	0	0
3	H	20	0	28	0	0
4	A	13	0	18	0	0
4	B	26	0	36	2	0
4	G	13	0	18	0	0
5	A	21	0	30	1	0
5	B	14	0	20	0	0
5	E	7	0	10	0	0
5	F	7	0	10	0	0
5	G	14	0	20	0	0
5	H	7	0	10	0	0
6	A	6	0	8	1	0
7	E	8	0	12	0	0
8	A	263	0	0	0	0
8	B	236	0	0	1	0
8	C	176	0	0	0	0
8	D	148	0	0	0	0
8	E	280	0	0	0	0
8	F	243	0	0	1	0
8	G	221	0	0	0	0
8	H	213	0	0	0	0
All	All	22450	0	20806	78	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 2.

All (78) 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:219:VAL:HG11	1:C:230:LEU:HD12	1.66	0.77
1:D:219:VAL:HG11	1:D:230:LEU:HD12	1.69	0.73
1:B:219:VAL:HG11	1:B:230:LEU:HD12	1.72	0.72
1:D:86:LEU:HD13	1:D:88:TRP:CZ2	2.28	0.69
1:A:86:LEU:HD13	1:A:88:TRP:CZ2	2.30	0.66
1:B:86:LEU:HD13	1:B:88:TRP:CZ2	2.30	0.66
1:A:171:LEU:HD21	1:A:255:THR:HB	1.79	0.63
1:A:55:GLY:HA2	5:A:406:PEG:H32	1.81	0.63
1:G:206:MET:HA	1:G:206:MET:HE2	1.81	0.62
1:E:206[A]:MET:HE1	1:G:206:MET:SD	2.40	0.62
1:C:86:LEU:HD13	1:C:88:TRP:CZ2	2.37	0.60
1:F:86:LEU:HD13	1:F:88:TRP:CZ2	2.40	0.56
1:H:86:LEU:HD13	1:H:88:TRP:CZ2	2.39	0.56
4:B:408:PG4:H62	1:C:206[A]:MET:HE2	1.85	0.56
1:E:86:LEU:HD13	1:E:88:TRP:CZ2	2.41	0.56
1:D:160:LEU:HD22	1:D:178:MET:SD	2.46	0.56
1:C:5:VAL:HG22	1:C:95:VAL:HB	1.87	0.55
1:G:86:LEU:HD13	1:G:88:TRP:CZ2	2.40	0.55
1:E:219:VAL:HG11	1:E:230:LEU:HD12	1.89	0.55
1:H:2:THR:HG21	1:H:31:GLU:HG2	1.89	0.54
1:E:206[B]:MET:SD	1:G:206:MET:HE1	2.49	0.53
1:B:218:ALA:HB3	8:B:505:HOH:O	2.09	0.51
1:C:216:ALA:O	1:C:219:VAL:HG12	2.11	0.51
1:F:60:THR:HG22	8:F:712:HOH:O	2.12	0.50
1:D:216:ALA:O	1:D:219:VAL:HG12	2.12	0.50
1:B:286:ILE:HA	4:B:408:PG4:H12	1.95	0.49
1:H:10:TYR:CZ	1:H:15:ARG:HG2	2.50	0.47
1:C:160:LEU:HD22	1:C:178:MET:SD	2.54	0.47
1:G:139:ASN:O	1:G:142:VAL:HG22	2.13	0.47
1:H:83:PRO:HA	1:H:86:LEU:HD12	1.97	0.46
1:A:135:VAL:HG23	1:A:222:VAL:HG21	1.98	0.46
1:A:41:PRO:HB3	1:A:77:VAL:HG11	1.98	0.45
1:C:139:ASN:CG	1:C:222:VAL:HG13	2.40	0.45
1:D:83:PRO:HG2	1:D:111:ALA:HB3	1.99	0.45
1:C:135:VAL:HB	1:C:222:VAL:HG11	1.98	0.45
1:G:105:SER:OG	1:G:108:LYS:HG3	2.17	0.44
1:D:5:VAL:HG22	1:D:95:VAL:HB	1.98	0.44
1:B:174:GLU:HG2	1:B:252:LYS:HG2	1.98	0.44
1:H:10:TYR:CE2	1:H:15:ARG:HG2	2.52	0.44
1:E:244:LEU:HD11	1:E:312:SER:HB3	1.99	0.44
1:A:193:VAL:HG22	1:A:194:TYR:N	2.33	0.43
1:B:10:TYR:CE2	1:B:15:ARG:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:PRO:HA	1:F:86:LEU:HD12	2.00	0.43
1:C:83:PRO:HA	1:C:86:LEU:HD12	2.01	0.43
1:C:10:TYR:CZ	1:C:15:ARG:HG2	2.54	0.43
1:A:301:LEU:CD2	6:A:405:GOL:H2	2.49	0.43
1:B:193:VAL:HG22	1:B:194:TYR:N	2.34	0.43
1:B:41:PRO:HB3	1:B:77:VAL:HG11	2.00	0.42
1:F:10:TYR:CE2	1:F:15:ARG:HG2	2.54	0.42
1:B:40:ASP:OD2	1:B:42:LYS:HB2	2.20	0.42
1:F:180:THR:O	1:F:180:THR:HG23	2.18	0.42
1:G:88:TRP:HA	1:G:88:TRP:CE3	2.54	0.42
1:E:161:ALA:HB3	1:E:162:PRO:HD3	2.01	0.42
1:E:10:TYR:CZ	1:E:15:ARG:HG2	2.55	0.42
1:B:43:THR:HG23	1:D:198:LEU:CD2	2.49	0.41
1:A:310:LYS:HB2	1:D:177:LEU:HD13	2.03	0.41
1:B:310:LYS:HB2	1:C:177:LEU:HD13	2.02	0.41
1:G:161:ALA:HB3	1:G:162:PRO:HD3	2.03	0.41
1:D:161:ALA:HB3	1:D:162:PRO:HD3	2.02	0.41
1:E:43:THR:HG23	1:H:198:LEU:CD2	2.50	0.41
1:A:139:ASN:O	1:A:142:VAL:HG22	2.20	0.41
1:F:206:MET:HE1	1:H:206:MET:SD	2.61	0.41
1:B:83:PRO:HA	1:B:86:LEU:HD12	2.03	0.41
1:F:286:ILE:HD13	1:H:52:THR:HG23	2.03	0.41
1:B:180[A]:THR:HG23	1:B:234:ALA:CB	2.50	0.41
1:E:286:ILE:HD13	1:G:52:THR:HG23	2.03	0.41
1:A:180:THR:HG23	1:A:180:THR:O	2.21	0.40
1:D:193:VAL:HG22	1:D:194:TYR:N	2.36	0.40
1:G:88:TRP:HA	1:G:88:TRP:HE3	1.85	0.40
1:G:244:LEU:CD2	1:H:235:ILE:HD13	2.50	0.40
1:C:10:TYR:CE2	1:C:15:ARG:HG2	2.55	0.40
1:B:139:ASN:O	1:B:142:VAL:HG22	2.20	0.40
1:D:83:PRO:HG2	1:D:111:ALA:CB	2.52	0.40
1:D:182:HIS:HB3	1:D:236:ARG:HD3	2.02	0.40
1:E:245:VAL:O	1:E:312:SER:HA	2.21	0.40
1:F:165:LYS:HB3	1:F:166:PRO:HD3	2.03	0.40
1:G:127:GLY:O	1:G:130:VAL:HG22	2.21	0.40
1:C:291:ASN:HD21	3:C:402:PGE:H3	1.87	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	335/344 (97%)	325 (97%)	9 (3%)	1 (0%)	36	35
1	B	337/344 (98%)	329 (98%)	7 (2%)	1 (0%)	36	35
1	C	337/344 (98%)	328 (97%)	8 (2%)	1 (0%)	36	35
1	D	335/344 (97%)	326 (97%)	8 (2%)	1 (0%)	36	35
1	E	343/344 (100%)	334 (97%)	8 (2%)	1 (0%)	36	35
1	F	336/344 (98%)	326 (97%)	9 (3%)	1 (0%)	36	35
1	G	335/344 (97%)	325 (97%)	9 (3%)	1 (0%)	36	35
1	H	337/344 (98%)	327 (97%)	9 (3%)	1 (0%)	36	35
All	All	2695/2752 (98%)	2620 (97%)	67 (2%)	8 (0%)	36	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	B	242	VAL
1	C	242	VAL
1	D	242	VAL
1	E	242	VAL
1	F	242	VAL
1	G	242	VAL
1	H	242	VAL

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	278/286 (97%)	278 (100%)	0	100	100
1	B	280/286 (98%)	280 (100%)	0	100	100
1	C	277/286 (97%)	277 (100%)	0	100	100
1	D	274/286 (96%)	274 (100%)	0	100	100
1	E	280/286 (98%)	280 (100%)	0	100	100
1	F	277/286 (97%)	277 (100%)	0	100	100
1	G	275/286 (96%)	275 (100%)	0	100	100
1	H	278/286 (97%)	278 (100%)	0	100	100
All	All	2219/2288 (97%)	2219 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	168	HIS
1	F	241	ASN
1	F	289	ASN
1	H	241	ASN
1	H	289	ASN
1	H	296	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 37 ligands modelled in this entry, 12 are monoatomic - leaving 25 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	$\# Z > 2$
5	PEG	A	406	-	6,6,6	0.31	0	5,5,5	0.29	0
5	PEG	A	404	-	6,6,6	0.25	0	5,5,5	0.34	0
5	PEG	H	403	-	6,6,6	0.25	0	5,5,5	0.24	0
3	PGE	B	405	-	9,9,9	0.28	0	8,8,8	0.48	0
5	PEG	G	402	-	6,6,6	0.28	0	5,5,5	0.27	0
4	PG4	B	406	-	12,12,12	0.30	0	11,11,11	0.25	0
3	PGE	A	402	-	9,9,9	0.26	0	8,8,8	0.50	0
3	PGE	H	404	-	9,9,9	0.28	0	8,8,8	0.55	0
3	PGE	E	405	-	9,9,9	0.31	0	8,8,8	0.51	0
3	PGE	C	402	-	9,9,9	0.26	0	8,8,8	0.49	0
5	PEG	B	404	-	6,6,6	0.25	0	5,5,5	0.31	0
5	PEG	G	404	-	6,6,6	0.28	0	5,5,5	0.30	0
5	PEG	A	407	-	6,6,6	0.28	0	5,5,5	0.26	0
3	PGE	D	402	-	9,9,9	0.29	0	8,8,8	0.63	0
4	PG4	A	403	-	12,12,12	0.30	0	11,11,11	0.22	0
6	GOL	A	405	-	5,5,5	0.30	0	5,5,5	0.26	0
3	PGE	H	402	-	9,9,9	0.31	0	8,8,8	0.59	0
4	PG4	G	403	-	12,12,12	0.32	0	11,11,11	0.22	0
7	TRS	E	404	-	7,7,7	0.38	0	9,9,9	0.75	0
3	PGE	F	403	-	9,9,9	0.29	0	8,8,8	0.62	0
4	PG4	B	408	-	12,12,12	0.32	0	11,11,11	0.24	0
5	PEG	E	403	-	6,6,6	0.30	0	5,5,5	0.16	0
5	PEG	F	404	-	6,6,6	0.34	0	5,5,5	0.31	0
3	PGE	B	409	-	9,9,9	0.30	0	8,8,8	0.52	0
5	PEG	B	407	-	6,6,6	0.28	0	5,5,5	0.19	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
5	PEG	A	406	-	-	3/4/4/4	-
5	PEG	A	404	-	-	1/4/4/4	-
5	PEG	H	403	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	B	405	-	-	4/7/7/7	-
5	PEG	G	402	-	-	0/4/4/4	-
4	PG4	B	406	-	-	4/10/10/10	-
3	PGE	A	402	-	-	2/7/7/7	-
3	PGE	H	404	-	-	4/7/7/7	-
3	PGE	E	405	-	-	2/7/7/7	-
3	PGE	C	402	-	-	3/7/7/7	-
5	PEG	B	404	-	-	0/4/4/4	-
5	PEG	G	404	-	-	3/4/4/4	-
5	PEG	A	407	-	-	4/4/4/4	-
3	PGE	D	402	-	-	4/7/7/7	-
4	PG4	A	403	-	-	4/10/10/10	-
6	GOL	A	405	-	-	0/4/4/4	-
3	PGE	H	402	-	-	3/7/7/7	-
4	PG4	G	403	-	-	2/10/10/10	-
7	TRS	E	404	-	-	0/9/9/9	-
3	PGE	F	403	-	-	2/7/7/7	-
4	PG4	B	408	-	-	3/10/10/10	-
5	PEG	E	403	-	-	1/4/4/4	-
5	PEG	F	404	-	-	0/4/4/4	-
3	PGE	B	409	-	-	3/7/7/7	-
5	PEG	B	407	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	405	PGE	O2-C3-C4-O3
4	B	406	PG4	O2-C3-C4-O3
4	B	408	PG4	O2-C3-C4-O3
4	A	403	PG4	O3-C5-C6-O4
4	A	403	PG4	O2-C3-C4-O3
3	F	403	PGE	O2-C3-C4-O3
4	B	406	PG4	O3-C5-C6-O4
3	A	402	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	G	403	PG4	O1-C1-C2-O2
5	A	406	PEG	O2-C3-C4-O4
3	B	405	PGE	O3-C5-C6-O4
3	C	402	PGE	O1-C1-C2-O2
3	H	404	PGE	O3-C5-C6-O4
5	A	406	PEG	O1-C1-C2-O2
3	D	402	PGE	O1-C1-C2-O2
3	H	402	PGE	O1-C1-C2-O2
3	D	402	PGE	O3-C5-C6-O4
5	A	407	PEG	O1-C1-C2-O2
3	H	404	PGE	O2-C3-C4-O3
4	B	406	PG4	O1-C1-C2-O2
4	B	408	PG4	O1-C1-C2-O2
5	A	404	PEG	O1-C1-C2-O2
5	B	407	PEG	O2-C3-C4-O4
3	E	405	PGE	O2-C3-C4-O3
3	C	402	PGE	O3-C5-C6-O4
5	G	404	PEG	O2-C3-C4-O4
5	A	407	PEG	C4-C3-O2-C2
3	H	402	PGE	C6-C5-O3-C4
3	H	402	PGE	C3-C4-O3-C5
5	A	407	PEG	C1-C2-O2-C3
3	B	409	PGE	C3-C4-O3-C5
3	C	402	PGE	C6-C5-O3-C4
3	B	409	PGE	O2-C3-C4-O3
3	D	402	PGE	C6-C5-O3-C4
3	F	403	PGE	O1-C1-C2-O2
5	E	403	PEG	C4-C3-O2-C2
5	G	404	PEG	C4-C3-O2-C2
3	A	402	PGE	C1-C2-O2-C3
3	H	404	PGE	C6-C5-O3-C4
5	H	403	PEG	O1-C1-C2-O2
5	B	407	PEG	C1-C2-O2-C3
5	G	404	PEG	O1-C1-C2-O2
3	B	405	PGE	C3-C4-O3-C5
3	H	404	PGE	O1-C1-C2-O2
5	A	407	PEG	O2-C3-C4-O4
4	B	406	PG4	C5-C6-O4-C7
5	A	406	PEG	C4-C3-O2-C2
4	A	403	PG4	O4-C7-C8-O5
4	G	403	PG4	O3-C5-C6-O4
3	D	402	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
3	E	405	PGE	C6-C5-O3-C4
3	B	405	PGE	C4-C3-O2-C2
4	A	403	PG4	C3-C4-O3-C5
3	B	409	PGE	O1-C1-C2-O2
4	B	408	PG4	O3-C5-C6-O4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	PEG	1	0
3	C	402	PGE	1	0
6	A	405	GOL	1	0
4	B	408	PG4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/344 (97%)	-0.35	2 (0%) 85 85	12, 25, 39, 60	1 (0%)
1	B	336/344 (97%)	-0.32	3 (0%) 81 80	13, 25, 39, 64	3 (0%)
1	C	336/344 (97%)	0.10	3 (0%) 81 80	12, 39, 62, 86	3 (0%)
1	D	336/344 (97%)	0.16	1 (0%) 90 89	19, 40, 64, 80	1 (0%)
1	E	343/344 (99%)	-0.20	7 (2%) 65 64	16, 28, 45, 81	2 (0%)
1	F	336/344 (97%)	-0.17	2 (0%) 85 85	16, 31, 44, 69	2 (0%)
1	G	336/344 (97%)	0.01	3 (0%) 81 80	19, 35, 49, 65	1 (0%)
1	H	338/344 (98%)	0.04	4 (1%) 76 76	17, 35, 51, 72	1 (0%)
All	All	2697/2752 (98%)	-0.09	25 (0%) 81 80	12, 32, 55, 86	14 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	-6	ALA	3.7
1	C	1	MET	3.6
1	E	-3	HIS	3.2
1	H	0	HIS	3.0
1	G	1	MET	3.0
1	H	-1	HIS	2.8
1	D	1	MET	2.8
1	F	38	LEU	2.7
1	F	1	MET	2.7
1	E	196	GLU	2.6
1	G	27	LYS	2.5
1	H	170	LYS	2.5
1	E	-1	HIS	2.4
1	A	1	MET	2.4
1	B	218	ALA	2.4
1	C	25	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	1	MET	2.3
1	A	40	ASP	2.2
1	G	24	ASN	2.2
1	B	40	ASP	2.2
1	E	58	PRO	2.1
1	E	213	THR	2.1
1	E	-4	HIS	2.1
1	B	1	MET	2.1
1	C	213	THR	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
2	MG	F	401	1/1	0.74	0.11	63,63,63,63	0
4	PG4	B	408	13/13	0.74	0.19	31,46,54,54	0
6	GOL	A	405	6/6	0.74	0.25	44,50,58,62	0
3	PGE	D	402	10/10	0.75	0.16	45,48,54,57	0
5	PEG	A	407	7/7	0.79	0.16	50,54,60,64	0
5	PEG	G	404	7/7	0.79	0.16	47,54,61,70	0
3	PGE	H	402	10/10	0.79	0.18	38,50,61,63	0
3	PGE	H	404	10/10	0.80	0.14	48,53,59,62	0
2	MG	D	401	1/1	0.82	0.15	70,70,70,70	0
3	PGE	C	402	10/10	0.83	0.14	43,49,54,60	0
3	PGE	E	405	10/10	0.83	0.15	36,42,49,52	0
5	PEG	H	403	7/7	0.84	0.15	38,45,50,53	0
3	PGE	B	405	10/10	0.84	0.15	30,37,47,52	0
3	PGE	F	403	10/10	0.85	0.14	36,46,52,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	G	403	13/13	0.85	0.14	34,40,57,58	0
5	PEG	A	406	7/7	0.86	0.14	26,28,45,48	0
3	PGE	A	402	10/10	0.86	0.13	29,33,40,41	0
5	PEG	F	404	7/7	0.86	0.13	37,44,46,54	0
5	PEG	B	407	7/7	0.87	0.13	34,38,50,51	0
4	PG4	B	406	13/13	0.88	0.12	42,53,63,63	0
2	MG	C	401	1/1	0.88	0.08	66,66,66,66	0
4	PG4	A	403	13/13	0.89	0.11	34,48,55,56	0
5	PEG	A	404	7/7	0.89	0.10	40,41,48,49	0
5	PEG	G	402	7/7	0.89	0.12	42,42,48,49	0
3	PGE	B	409	10/10	0.91	0.10	25,41,48,49	0
5	PEG	B	404	7/7	0.91	0.11	30,37,43,43	0
2	MG	H	401	1/1	0.93	0.07	50,50,50,50	0
5	PEG	E	403	7/7	0.94	0.09	29,37,42,44	0
2	MG	A	401	1/1	0.94	0.05	42,42,42,42	0
2	MG	G	401	1/1	0.95	0.04	29,29,29,29	0
7	TRS	E	404	8/8	0.95	0.06	26,33,36,37	0
2	MG	E	401	1/1	0.96	0.05	50,50,50,50	0
2	MG	B	403	1/1	0.96	0.05	46,46,46,46	0
2	MG	F	402	1/1	0.96	0.04	30,30,30,30	0
2	MG	B	401	1/1	0.97	0.05	42,42,42,42	0
2	MG	E	402	1/1	0.98	0.06	38,38,38,38	0
2	MG	B	402	1/1	0.98	0.03	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.