



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:36 PM UTC

PDB ID : 6I34 / pdb_00006i34
Title : Crystal structure of Neanderthal glycine decarboxylase (P-protein)
Authors : Van Laer, B.; Kapp, U.; Leonard, G.; Mueller-Dieckmann, C.
Deposited on : 2018-11-05
Resolution : 2.10 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

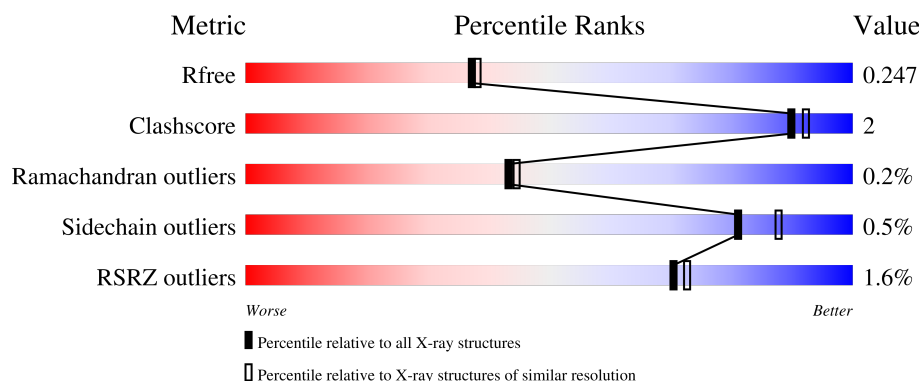
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	984	% 92% ...
1	B	984	2% 92% ...
1	C	984	2% 91% 5% ..
1	D	984	% 91% 5% .

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	EDO	C	1102	-	-	X	-
4	PEG	A	1105	-	-	X	-
4	PEG	C	1106	-	-	X	-

2 Entry composition [i](#)

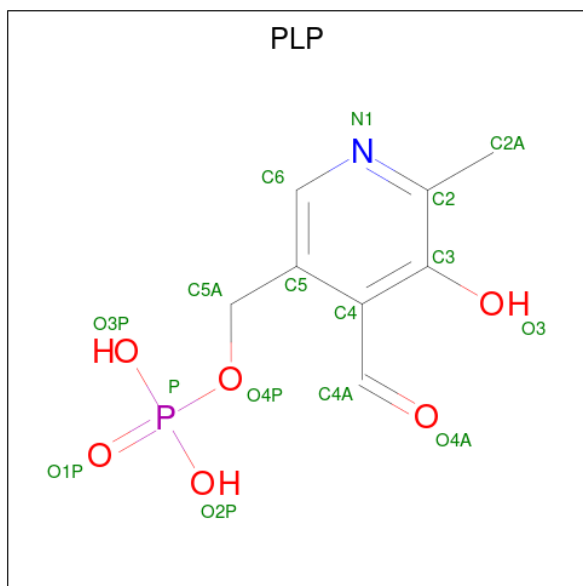
There are 6 unique types of molecules in this entry. The entry contains 31302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Neanderthal Glycine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	2	0
			7450	4694	1319	1382	55			
1	B	954	Total	C	N	O	S	0	1	0
			7454	4696	1320	1384	54			
1	C	953	Total	C	N	O	S	0	0	0
			7436	4687	1317	1378	54			
1	D	953	Total	C	N	O	S	0	0	0
			7434	4685	1314	1381	54			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



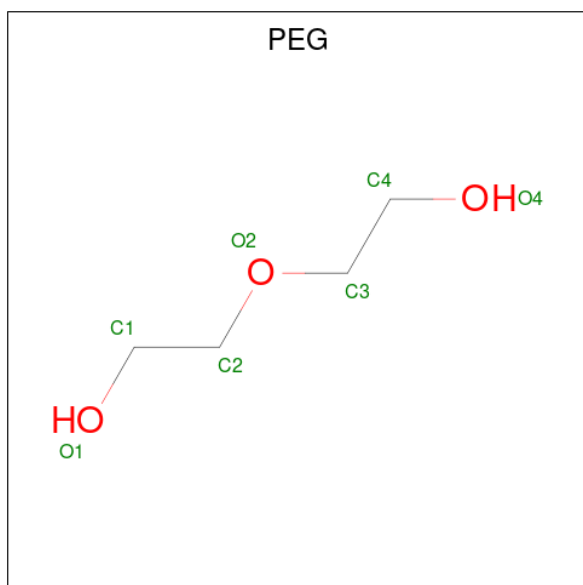
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

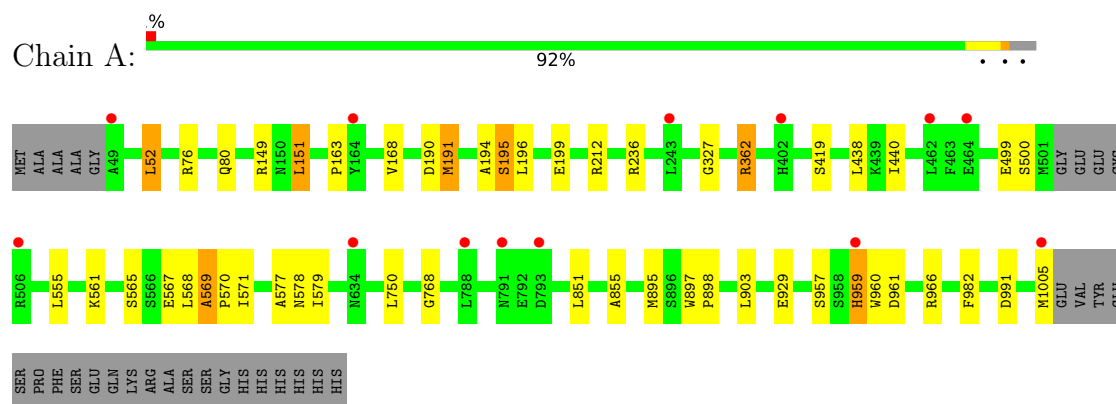
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	403	Total	O	0	0
			403	403		
6	B	282	Total	O	0	0
			282	282		
6	C	404	Total	O	0	0
			404	404		
6	D	270	Total	O	0	0
			270	270		

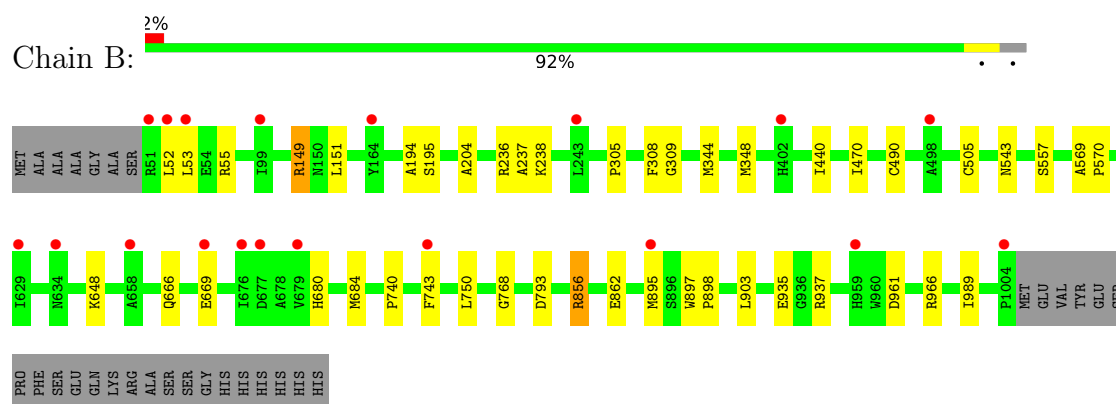
3 Residue-property plots [i](#)

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.

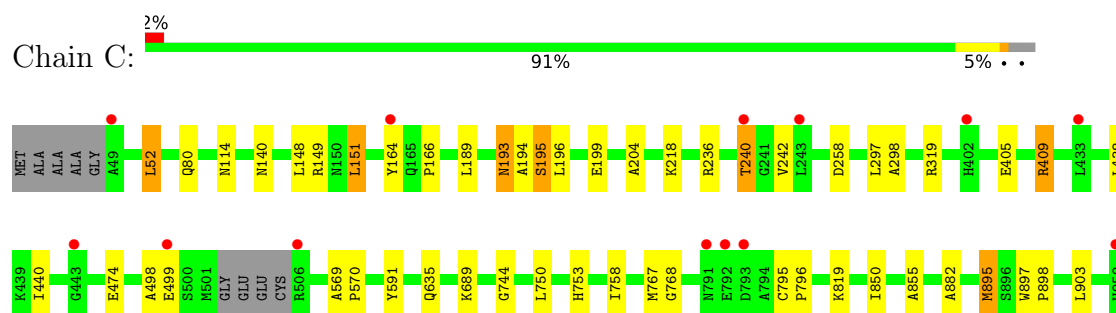
• Molecule 1: Neanderthal Glycine decarboxylase

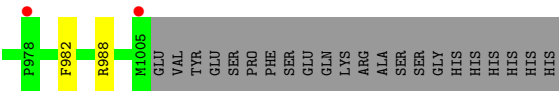


• Molecule 1: Neanderthal Glycine decarboxylase

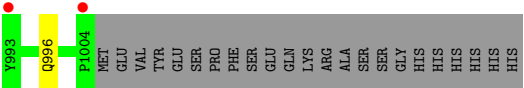
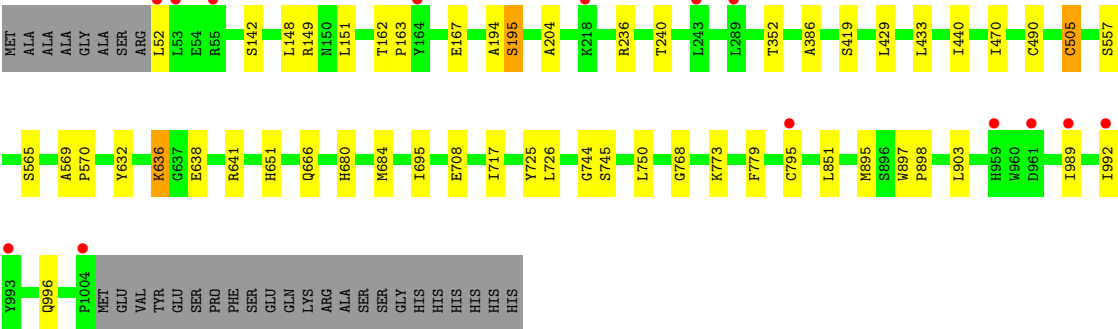
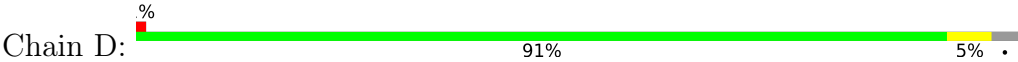


• Molecule 1: Neanderthal Glycine decarboxylase





● Molecule 1: Neanderthal Glycine decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.87Å 124.38Å 201.30Å 90.00° 98.57° 90.00°	Depositor
Resolution (Å)	47.90 – 2.10 47.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.90-2.10) 99.8 (47.90-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.216 , 0.243 0.223 , 0.247	Depositor DCC
R_{free} test set	12263 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	31302	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.09 % 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 3.9183e-06. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, PEG, PLP, 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	1.16	12/7617 (0.2%)	1.03	14/10316 (0.1%)
1	B	1.06	2/7622 (0.0%)	1.00	8/10323 (0.1%)
1	C	1.16	12/7603 (0.2%)	1.02	9/10296 (0.1%)
1	D	1.09	3/7602 (0.0%)	1.01	9/10297 (0.1%)
All	All	1.12	29/30444 (0.1%)	1.01	40/41232 (0.1%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	151	LEU	CA-C	6.32	1.57	1.52
1	C	298	ALA	C-O	-6.27	1.16	1.24
1	D	167	GLU	C-O	-6.19	1.16	1.24
1	D	149	ARG	C-O	-6.05	1.17	1.24
1	A	569	ALA	C-O	-5.91	1.18	1.24
1	A	579	ILE	C-O	-5.81	1.17	1.24
1	A	168	VAL	C-O	-5.79	1.17	1.24
1	C	795	CYS	C-O	-5.68	1.17	1.24
1	C	819	LYS	C-O	5.63	1.31	1.24
1	A	52	LEU	C-O	-5.61	1.17	1.24
1	D	851	LEU	C-O	-5.60	1.17	1.24
1	C	193	ASN	C-O	-5.58	1.16	1.23
1	A	567	GLU	C-O	-5.53	1.17	1.24
1	C	52	LEU	C-O	-5.53	1.17	1.24
1	A	191	MET	C-O	-5.53	1.17	1.23
1	A	236	ARG	C-O	-5.53	1.17	1.24
1	A	151	LEU	CA-C	5.49	1.57	1.52
1	C	796	PRO	C-O	-5.43	1.17	1.23
1	C	194	ALA	C-O	-5.42	1.16	1.24
1	A	561	LYS	CA-C	5.38	1.60	1.53
1	C	591	TYR	C-O	-5.27	1.18	1.24
1	A	327	GLY	C-O	5.23	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	LEU	C-O	-5.13	1.18	1.24
1	C	498	ALA	C-O	-5.13	1.18	1.24
1	C	988	ARG	C-O	-5.12	1.17	1.23
1	A	555	LEU	N-CA	-5.09	1.39	1.46
1	B	862	GLU	CA-C	5.09	1.58	1.52
1	A	929	GLU	N-CA	5.03	1.52	1.46
1	C	635	GLN	C-O	-5.02	1.17	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	851	LEU	N-CA-C	7.85	119.47	111.07
1	D	708	GLU	N-CA-C	7.31	119.25	111.28
1	B	966	ARG	NE-CZ-NH2	7.30	125.77	119.20
1	A	190	ASP	N-CA-C	7.01	120.31	111.69
1	A	163	PRO	CA-C-N	6.88	130.06	120.29
1	A	163	PRO	C-N-CA	6.88	130.06	120.29
1	C	850	ILE	N-CA-C	-6.76	98.53	108.54
1	B	961	ASP	N-CA-C	6.74	120.95	111.52
1	B	194	ALA	CA-C-N	6.59	134.13	121.54
1	B	194	ALA	C-N-CA	6.59	134.13	121.54
1	A	194	ALA	CA-C-N	6.55	134.05	121.54
1	A	194	ALA	C-N-CA	6.55	134.05	121.54
1	C	194	ALA	CA-C-N	6.55	134.05	121.54
1	C	194	ALA	C-N-CA	6.55	134.05	121.54
1	A	577	ALA	N-CA-C	6.55	119.42	111.82
1	B	490	CYS	N-CA-C	6.53	120.51	112.54
1	D	194	ALA	CA-C-N	6.49	133.94	121.54
1	D	194	ALA	C-N-CA	6.49	133.94	121.54
1	D	490	CYS	N-CA-C	6.28	119.10	111.82
1	B	793	ASP	N-CA-C	6.19	120.39	112.34
1	C	895	MET	N-CA-C	5.64	118.16	109.07
1	D	744	GLY	N-CA-C	5.61	123.08	115.00
1	A	199	GLU	N-CA-C	5.58	117.04	111.07
1	C	195	SER	N-CA-CB	5.57	119.90	110.49
1	D	505	CYS	CB-CA-C	5.56	118.90	109.84
1	B	149	ARG	N-CA-C	5.49	117.07	111.14
1	D	386	ALA	N-CA-C	5.45	117.64	111.11
1	C	744	GLY	N-CA-C	5.44	122.62	114.95
1	A	855	ALA	N-CA-C	5.36	117.88	111.71
1	A	578	ASN	N-CA-C	5.36	120.07	111.81
1	A	212	ARG	NE-CZ-NH1	-5.35	116.15	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	GLU	N-CA-C	5.34	116.78	111.07
1	C	689	LYS	N-CA-C	5.20	118.40	111.75
1	D	195	SER	N-CA-C	5.19	121.85	110.80
1	C	855	ALA	N-CA-C	5.14	117.56	111.33
1	B	309	GLY	N-CA-C	5.10	125.28	113.18
1	A	568	LEU	N-CA-C	5.06	116.87	111.36
1	A	149	ARG	N-CA-C	5.06	116.60	111.14
1	D	636	LYS	N-CA-CB	-5.05	103.14	110.47
1	A	195	SER	N-CA-C	5.03	121.52	110.80

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	7450	0	7375	17	0
1	B	7454	0	7376	26	0
1	C	7436	0	7367	31	0
1	D	7434	0	7356	34	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	6	0	0
2	D	15	0	7	0	0
3	A	12	0	18	0	0
3	B	12	0	18	0	0
3	C	12	0	18	5	0
3	D	8	0	12	0	0
4	A	7	0	10	5	0
4	B	7	0	10	1	0
4	C	14	0	20	6	0
4	D	7	0	10	0	0
5	A	12	0	16	0	0
5	C	12	0	16	0	0
5	D	6	0	8	1	0
6	A	403	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	282	0	0	0	0
6	C	404	0	0	2	0
6	D	270	0	0	0	0
All	All	31302	0	29655	108	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 (108) 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:856:ARG:HH11	1:B:856:ARG:HG3	1.11	1.15
1:C:474:GLU:HB2	3:C:1102:EDO:H11	1.36	1.01
1:B:680:HIS:HE2	1:B:684:MET:HE2	1.37	0.90
1:D:680:HIS:HE2	1:D:684:MET:HE2	1.39	0.87
1:C:895:MET:SD	1:C:903:LEU:HD22	2.15	0.86
1:C:319:ARG:HB2	3:C:1102:EDO:H21	1.61	0.82
1:C:882:ALA:HB2	1:C:895:MET:HE2	1.66	0.78
1:C:114:ASN:HB3	4:C:1106:PEG:H12	1.67	0.77
1:B:856:ARG:HG3	1:B:856:ARG:NH1	1.91	0.77
1:D:680:HIS:NE2	1:D:684:MET:HE2	2.01	0.76
1:C:297:LEU:HD22	3:C:1102:EDO:H12	1.68	0.75
1:B:680:HIS:NE2	1:B:684:MET:HE2	2.01	0.74
1:C:895:MET:SD	1:C:903:LEU:CD2	2.76	0.74
1:C:895:MET:HE1	1:C:903:LEU:HD21	1.71	0.72
1:D:895:MET:SD	1:D:903:LEU:HD22	2.33	0.68
1:B:895:MET:SD	1:B:903:LEU:HD22	2.36	0.66
1:B:344:MET:HE3	1:B:348:MET:CE	2.26	0.66
1:B:935:GLU:HG3	1:B:937:ARG:HH21	1.60	0.65
1:A:362:ARG:NE	1:A:991:ASP:OD1	2.28	0.65
1:A:895:MET:SD	1:A:903:LEU:HD22	2.36	0.64
4:A:1105:PEG:H11	1:B:543:ASN:HD22	1.63	0.63
4:A:1105:PEG:H41	6:A:1549:HOH:O	1.99	0.62
1:A:982:PHE:HD2	4:A:1105:PEG:H31	1.65	0.62
1:B:740:PRO:HA	1:B:743:PHE:CE2	2.36	0.61
1:C:474:GLU:CB	3:C:1102:EDO:H11	2.22	0.59
1:C:114:ASN:CB	4:C:1106:PEG:H12	2.33	0.59
1:D:895:MET:SD	1:D:903:LEU:CD2	2.91	0.59
1:B:895:MET:SD	1:B:903:LEU:CD2	2.92	0.58
1:B:52:LEU:HD23	1:B:55:ARG:HD2	1.86	0.58
1:A:895:MET:SD	1:A:903:LEU:CD2	2.92	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:MET:HE1	6:A:1391:HOH:O	2.03	0.57
1:B:344:MET:HE3	1:B:348:MET:HE3	1.84	0.57
1:D:148:LEU:C	1:D:148:LEU:HD23	2.30	0.57
1:C:895:MET:HE1	1:C:903:LEU:CD2	2.34	0.57
1:A:499:GLU:HG2	1:B:52:LEU:HD12	1.87	0.56
1:D:352:THR:CG2	1:D:989:ILE:HD11	2.35	0.56
4:A:1105:PEG:H42	6:A:1456:HOH:O	2.06	0.56
1:A:982:PHE:CD2	4:A:1105:PEG:H31	2.42	0.55
1:D:162:THR:CG2	1:D:163:PRO:HD2	2.37	0.55
1:D:162:THR:HG22	1:D:163:PRO:HD2	1.89	0.54
1:B:204:ALA:HB1	1:B:236:ARG:HG2	1.91	0.53
1:D:352:THR:HG23	1:D:989:ILE:HD11	1.91	0.52
1:A:569:ALA:HB3	1:A:570:PRO:HD3	1.92	0.51
1:C:499:GLU:HA	1:D:52:LEU:HD23	1.91	0.51
1:D:666:GLN:OE1	1:D:684:MET:HE3	2.10	0.51
1:B:666:GLN:OE1	1:B:684:MET:HE3	2.11	0.50
4:C:1105:PEG:H12	6:C:1452:HOH:O	2.10	0.50
1:D:632:TYR:OH	1:D:636:LYS:NZ	2.30	0.50
1:C:895:MET:CE	1:C:903:LEU:CD2	2.89	0.50
1:D:569:ALA:HB3	1:D:570:PRO:HD3	1.94	0.49
1:B:569:ALA:HB3	1:B:570:PRO:HD3	1.95	0.49
1:C:982:PHE:CD2	4:C:1105:PEG:H11	2.48	0.49
1:C:897:TRP:CD1	1:C:898:PRO:HA	2.48	0.49
1:B:440:ILE:CD1	1:B:470:ILE:HD12	2.43	0.49
1:A:897:TRP:CD1	1:A:898:PRO:HA	2.48	0.48
1:D:440:ILE:CD1	1:D:470:ILE:HD12	2.43	0.48
1:D:992:ILE:HG22	1:D:996:GLN:OE1	2.13	0.48
1:B:856:ARG:HH11	1:B:856:ARG:CG	2.01	0.48
1:B:305:PRO:HA	1:B:308:PHE:CE1	2.50	0.47
4:C:1106:PEG:C1	1:D:142:SER:HB3	2.44	0.47
1:D:745:SER:O	1:D:773:LYS:NZ	2.48	0.47
1:D:897:TRP:CD1	1:D:898:PRO:HA	2.50	0.47
1:B:897:TRP:CD1	1:B:898:PRO:HA	2.49	0.47
1:D:419:SER:OG	1:D:429:LEU:HD11	2.15	0.47
1:A:438:LEU:HB3	1:A:440:ILE:HD11	1.98	0.46
4:C:1106:PEG:H12	1:D:142:SER:HB3	1.97	0.46
1:B:750:LEU:O	1:B:768:GLY:HA2	2.15	0.45
1:B:740:PRO:HA	1:B:743:PHE:CZ	2.51	0.45
1:C:149:ARG:HD3	1:D:565:SER:OG	2.16	0.45
1:C:569:ALA:HB3	1:C:570:PRO:HD3	1.97	0.45
1:C:240:THR:HG22	1:C:242:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:TYR:C	1:D:725:TYR:CD1	2.95	0.45
1:A:959:HIS:NE2	1:A:961:ASP:OD2	2.50	0.44
1:C:767:MET:HE3	6:C:1258:HOH:O	2.17	0.44
1:C:882:ALA:HB2	1:C:895:MET:CE	2.41	0.44
1:C:204:ALA:HB1	1:C:236:ARG:HG2	1.98	0.44
1:C:164:TYR:O	1:C:166:PRO:HD3	2.17	0.44
1:C:218:LYS:HB2	1:C:258:ASP:O	2.17	0.44
1:D:433:LEU:HD12	1:D:433:LEU:HA	1.85	0.44
1:A:750:LEU:O	1:A:768:GLY:HA2	2.18	0.43
1:A:565:SER:OG	1:B:149:ARG:HD2	2.18	0.43
1:C:750:LEU:O	1:C:768:GLY:HA2	2.18	0.43
1:D:750:LEU:O	1:D:768:GLY:HA2	2.18	0.43
1:D:651:HIS:NE2	5:D:1105:GOL:H11	2.34	0.43
1:B:648:LYS:HE3	1:B:669:GLU:HG2	2.01	0.43
1:C:193:ASN:HD21	1:C:196:LEU:HG	1.84	0.42
6:A:1549:HOH:O	4:B:1105:PEG:H12	2.18	0.42
1:D:779:PHE:HA	1:D:795:CYS:O	2.19	0.42
1:A:151:LEU:C	1:A:151:LEU:HD23	2.44	0.42
1:C:148:LEU:C	1:C:148:LEU:HD23	2.44	0.42
1:D:726:LEU:C	1:D:726:LEU:HD23	2.44	0.42
1:C:140:ASN:O	3:C:1102:EDO:H22	2.19	0.42
1:D:996:GLN:HE21	1:D:996:GLN:HB3	1.71	0.42
1:C:151:LEU:C	1:C:151:LEU:HD23	2.44	0.41
1:D:151:LEU:C	1:D:151:LEU:HD23	2.45	0.41
1:A:957:SER:O	1:A:966:ARG:NH2	2.43	0.41
1:D:641:ARG:HH11	1:D:641:ARG:HG2	1.85	0.41
1:A:196:LEU:HD23	1:A:196:LEU:HA	1.81	0.41
1:D:240:THR:HG22	1:D:240:THR:O	2.20	0.41
1:D:204:ALA:HB1	1:D:236:ARG:HG2	2.02	0.41
1:C:438:LEU:HB3	1:C:440:ILE:HD11	2.01	0.41
1:B:151:LEU:HD23	1:B:151:LEU:C	2.46	0.41
1:C:405:GLU:O	1:C:409:ARG:HB2	2.21	0.41
1:A:76:ARG:O	1:A:80:GLN:HG3	2.21	0.40
1:C:753:HIS:HA	1:C:758:ILE:HB	2.02	0.40
1:B:237:ALA:O	1:B:238:LYS:C	2.64	0.40
1:D:638:GLU:HB3	1:D:641:ARG:HD2	2.03	0.40
1:D:695:ILE:CG2	1:D:717:ILE:HG12	2.51	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	951/984 (97%)	923 (97%)	25 (3%)	3 (0%)	36	36
1	B	953/984 (97%)	926 (97%)	26 (3%)	1 (0%)	48	50
1	C	949/984 (96%)	925 (98%)	23 (2%)	1 (0%)	48	50
1	D	951/984 (97%)	925 (97%)	25 (3%)	1 (0%)	48	50
All	All	3804/3936 (97%)	3699 (97%)	99 (3%)	6 (0%)	43	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	SER
1	B	195	SER
1	C	195	SER
1	D	195	SER
1	A	959	HIS
1	A	960	TRP

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	807/829 (97%)	801 (99%)	6 (1%)	76	83
1	B	807/829 (97%)	803 (100%)	4 (0%)	81	88
1	C	805/829 (97%)	800 (99%)	5 (1%)	78	86
1	D	805/829 (97%)	803 (100%)	2 (0%)	87	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3224/3316 (97%)	3207 (100%)	17 (0%)	81	88

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	191	MET
1	A	362	ARG
1	A	419	SER
1	A	500	SER
1	A	571	ILE
1	B	505	CYS
1	B	557	SER
1	B	856	ARG
1	B	989	ILE
1	C	52	LEU
1	C	80	GLN
1	C	189	LEU
1	C	240	THR
1	C	409	ARG
1	D	505	CYS
1	D	557	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	620	GLN
1	A	640	HIS
1	A	666	GLN
1	A	691	ASN
1	B	114	ASN
1	B	399	HIS
1	B	441	GLN
1	B	589	GLN
1	B	610	GLN
1	B	620	GLN
1	B	640	HIS
1	B	723	GLN
1	C	114	ASN
1	C	441	GLN

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Mol	Chain	Res	Type
1	C	620	GLN
1	C	666	GLN
1	C	691	ASN
1	C	791	ASN
1	C	847	HIS
1	C	928	GLN
1	D	114	ASN
1	D	441	GLN
1	D	589	GLN
1	D	620	GLN
1	D	640	HIS
1	D	723	GLN
1	D	928	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](#)

25 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	C	1103	-	3,3,3	0.59	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	A	1101	1	15,15,16	2.39	3 (20%)	21,22,23	2.12	4 (19%)
3	EDO	C	1102	-	3,3,3	0.52	0	2,2,2	0.74	0
4	PEG	C	1105	-	6,6,6	0.58	0	5,5,5	1.37	0
3	EDO	D	1103	-	3,3,3	0.89	0	2,2,2	0.95	0
4	PEG	D	1101	-	6,6,6	0.74	0	5,5,5	0.88	0
4	PEG	A	1105	-	6,6,6	0.55	0	5,5,5	0.56	0
4	PEG	C	1106	-	6,6,6	0.54	0	5,5,5	0.70	0
5	GOL	C	1108	-	5,5,5	0.88	0	5,5,5	1.23	0
3	EDO	C	1104	-	3,3,3	0.85	0	2,2,2	0.51	0
4	PEG	B	1105	-	6,6,6	0.69	0	5,5,5	0.71	0
3	EDO	B	1102	-	3,3,3	0.49	0	2,2,2	0.32	0
3	EDO	A	1104	-	3,3,3	0.37	0	2,2,2	0.53	0
5	GOL	A	1107	-	5,5,5	0.24	0	5,5,5	0.77	0
3	EDO	A	1102	-	3,3,3	0.75	0	2,2,2	0.33	0
3	EDO	B	1104	-	3,3,3	0.33	0	2,2,2	0.58	0
2	PLP	B	1101	1	15,15,16	3.37	3 (20%)	21,22,23	1.93	5 (23%)
3	EDO	A	1103	-	3,3,3	0.53	0	2,2,2	0.41	0
2	PLP	D	1102	1	15,15,16	3.46	3 (20%)	21,22,23	2.00	6 (28%)
3	EDO	D	1104	-	3,3,3	0.62	0	2,2,2	0.16	0
5	GOL	C	1107	-	5,5,5	0.31	0	5,5,5	0.33	0
5	GOL	D	1105	-	5,5,5	0.55	0	5,5,5	0.45	0
2	PLP	C	1101	1	15,15,16	2.87	4 (26%)	21,22,23	2.25	5 (23%)
3	EDO	B	1103	-	3,3,3	0.32	0	2,2,2	0.78	0
5	GOL	A	1106	-	5,5,5	0.62	0	5,5,5	0.98	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
3	EDO	C	1103	-	-	0/1/1/1	-
2	PLP	A	1101	1	-	2/6/6/8	0/1/1/1
3	EDO	C	1102	-	-	0/1/1/1	-
4	PEG	C	1105	-	-	3/4/4/4	-
3	EDO	D	1103	-	-	0/1/1/1	-
4	PEG	D	1101	-	-	3/4/4/4	-
4	PEG	A	1105	-	-	1/4/4/4	-
4	PEG	C	1106	-	-	3/4/4/4	-
5	GOL	C	1108	-	-	4/4/4/4	-
3	EDO	C	1104	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	1105	-	-	2/4/4/4	-
3	EDO	B	1102	-	-	1/1/1/1	-
3	EDO	A	1104	-	-	1/1/1/1	-
5	GOL	A	1107	-	-	2/4/4/4	-
3	EDO	A	1102	-	-	1/1/1/1	-
3	EDO	B	1104	-	-	1/1/1/1	-
2	PLP	B	1101	1	-	0/6/6/8	0/1/1/1
3	EDO	A	1103	-	-	1/1/1/1	-
2	PLP	D	1102	1	-	0/6/6/8	0/1/1/1
3	EDO	D	1104	-	-	0/1/1/1	-
5	GOL	C	1107	-	-	0/4/4/4	-
5	GOL	D	1105	-	-	4/4/4/4	-
2	PLP	C	1101	1	-	4/6/6/8	0/1/1/1
3	EDO	B	1103	-	-	1/1/1/1	-
5	GOL	A	1106	-	-	3/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	PLP	C3-C2	8.53	1.49	1.41
2	C	1101	PLP	C3-C2	8.43	1.49	1.41
2	D	1102	PLP	C3-C2	8.28	1.49	1.41
2	B	1101	PLP	C5-C4	8.22	1.49	1.40
2	D	1102	PLP	C5-C4	8.20	1.49	1.40
2	A	1101	PLP	C3-C2	6.00	1.47	1.41
2	D	1102	PLP	C3-C4	5.76	1.51	1.40
2	A	1101	PLP	C5-C4	5.60	1.46	1.40
2	C	1101	PLP	C5-C4	5.39	1.46	1.40
2	B	1101	PLP	C3-C4	4.66	1.49	1.40
2	A	1101	PLP	C3-C4	2.88	1.45	1.40
2	C	1101	PLP	C3-C4	2.67	1.45	1.40
2	C	1101	PLP	C6-C5	2.09	1.41	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	PLP	O4P-C5A-C5	6.00	120.60	109.36
2	C	1101	PLP	O2P-P-O4P	5.63	121.35	106.67
2	C	1101	PLP	O4P-C5A-C5	5.41	119.49	109.36
2	A	1101	PLP	O4P-P-O1P	4.78	119.36	106.44
2	D	1102	PLP	O3P-P-O4P	-4.41	95.16	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1102	PLP	O4P-C5A-C5	4.13	117.10	109.36
2	D	1102	PLP	O3P-P-O2P	4.02	122.88	107.80
2	B	1101	PLP	O4P-P-O1P	-3.99	95.64	106.44
2	B	1101	PLP	O4P-C5A-C5	3.98	116.81	109.36
2	C	1101	PLP	O3P-P-O4P	-3.17	98.40	106.67
2	B	1101	PLP	C4A-C4-C5	2.90	123.93	120.94
2	B	1101	PLP	C6-N1-C2	2.85	124.36	119.20
2	A	1101	PLP	O2P-P-O4P	-2.85	99.25	106.67
2	C	1101	PLP	C3-C4-C5	-2.67	115.39	118.59
2	D	1102	PLP	C6-N1-C2	2.52	123.77	119.20
2	A	1101	PLP	O3P-P-O4P	-2.29	100.70	106.67
2	C	1101	PLP	C4A-C4-C5	2.28	123.29	120.94
2	D	1102	PLP	O4P-P-O1P	2.19	112.37	106.44
2	D	1102	PLP	C3-C4-C5	-2.08	116.10	118.59
2	B	1101	PLP	O3P-P-O4P	2.06	112.04	106.67

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PLP	C4-C5-C5A-O4P
2	A	1101	PLP	C6-C5-C5A-O4P
2	C	1101	PLP	C4-C5-C5A-O4P
2	C	1101	PLP	C6-C5-C5A-O4P
2	C	1101	PLP	C5A-O4P-P-O1P
5	C	1108	GOL	O1-C1-C2-C3
5	C	1108	GOL	C1-C2-C3-O3
5	D	1105	GOL	O1-C1-C2-C3
4	C	1105	PEG	C4-C3-O2-C2
4	B	1105	PEG	O1-C1-C2-O2
4	C	1105	PEG	O1-C1-C2-O2
4	C	1105	PEG	O2-C3-C4-O4
4	C	1106	PEG	O1-C1-C2-O2
5	A	1106	GOL	O1-C1-C2-C3
5	A	1107	GOL	C1-C2-C3-O3
5	D	1105	GOL	C1-C2-C3-O3
5	A	1106	GOL	O1-C1-C2-O2
5	A	1107	GOL	O2-C2-C3-O3
5	C	1108	GOL	O1-C1-C2-O2
5	C	1108	GOL	O2-C2-C3-O3
5	D	1105	GOL	O1-C1-C2-O2
4	A	1105	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	1102	EDO	O1-C1-C2-O2
3	B	1102	EDO	O1-C1-C2-O2
3	C	1104	EDO	O1-C1-C2-O2
4	C	1106	PEG	O2-C3-C4-O4
4	D	1101	PEG	O1-C1-C2-O2
3	A	1104	EDO	O1-C1-C2-O2
4	D	1101	PEG	C1-C2-O2-C3
4	D	1101	PEG	C4-C3-O2-C2
3	A	1103	EDO	O1-C1-C2-O2
3	B	1103	EDO	O1-C1-C2-O2
4	B	1105	PEG	C4-C3-O2-C2
5	D	1105	GOL	O2-C2-C3-O3
4	C	1106	PEG	C4-C3-O2-C2
3	B	1104	EDO	O1-C1-C2-O2
2	C	1101	PLP	C5A-O4P-P-O3P
5	A	1106	GOL	O2-C2-C3-O3

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1102	EDO	5	0
4	C	1105	PEG	2	0
4	A	1105	PEG	5	0
4	C	1106	PEG	4	0
4	B	1105	PEG	1	0
5	D	1105	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	953/984 (96%)	0.03	13 (1%) 73 75	16, 29, 49, 81	2 (0%)
1	B	954/984 (96%)	0.40	19 (1%) 65 67	16, 41, 67, 99	1 (0%)
1	C	953/984 (96%)	0.05	15 (1%) 70 73	18, 29, 51, 97	0
1	D	953/984 (96%)	0.34	14 (1%) 72 74	21, 40, 64, 90	0
All	All	3813/3936 (96%)	0.21	61 (1%) 70 73	16, 34, 61, 99	3 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	6.7
1	D	52	LEU	6.0
1	A	959	HIS	5.2
1	C	959	HIS	4.6
1	C	49	ALA	3.9
1	A	791	ASN	3.8
1	D	1004	PRO	3.5
1	D	53	LEU	3.5
1	B	669	GLU	3.5
1	A	1005	MET	3.3
1	D	989	ILE	3.1
1	A	243	LEU	3.1
1	B	243	LEU	2.9
1	D	218	LYS	2.9
1	B	1004	PRO	2.9
1	B	634	ASN	2.9
1	C	164	TYR	2.8
1	B	676	ILE	2.8
1	B	53	LEU	2.7
1	C	792	GLU	2.7
1	B	164	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	791	ASN	2.7
1	A	793	ASP	2.6
1	C	1005	MET	2.6
1	B	959	HIS	2.6
1	A	49	ALA	2.6
1	C	243	LEU	2.5
1	B	679	VAL	2.5
1	B	895	MET	2.5
1	D	993	TYR	2.5
1	D	289	LEU	2.5
1	C	402	HIS	2.5
1	B	743	PHE	2.4
1	B	51	ARG	2.4
1	C	499	GLU	2.4
1	C	793	ASP	2.4
1	B	677	ASP	2.4
1	B	99	ILE	2.4
1	C	978	PRO	2.4
1	B	658	ALA	2.3
1	A	788	LEU	2.3
1	D	243	LEU	2.3
1	A	402	HIS	2.2
1	D	992	ILE	2.2
1	A	462	LEU	2.2
1	D	961	ASP	2.2
1	A	464	GLU	2.2
1	D	959	HIS	2.2
1	D	55	ARG	2.2
1	C	506	ARG	2.1
1	D	795	CYS	2.1
1	A	634	ASN	2.1
1	C	443	GLY	2.1
1	B	498	ALA	2.1
1	B	402	HIS	2.1
1	A	506	ARG	2.1
1	C	240	THR	2.1
1	A	164	TYR	2.0
1	D	164	TYR	2.0
1	B	629	ILE	2.0
1	C	433	LEU	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($\text{\AA}^2$)	Q<0.9
4	PEG	D	1101	7/7	0.70	0.23	38,41,63,65	0
3	EDO	B	1104	4/4	0.74	0.21	51,53,54,56	0
3	EDO	B	1103	4/4	0.74	0.23	44,50,50,53	0
4	PEG	A	1105	7/7	0.75	0.22	37,51,54,64	0
4	PEG	C	1105	7/7	0.76	0.21	37,43,48,53	0
5	GOL	D	1105	6/6	0.79	0.20	47,60,62,70	0
3	EDO	D	1104	4/4	0.80	0.21	33,37,46,50	0
3	EDO	C	1103	4/4	0.80	0.18	36,41,48,51	0
4	PEG	B	1105	7/7	0.80	0.16	36,39,45,49	0
3	EDO	A	1102	4/4	0.81	0.17	35,35,41,44	0
3	EDO	D	1103	4/4	0.81	0.23	38,41,42,56	0
3	EDO	A	1104	4/4	0.83	0.17	52,55,62,66	0
5	GOL	A	1107	6/6	0.83	0.15	40,51,52,56	0
3	EDO	B	1102	4/4	0.83	0.18	35,44,45,48	0
4	PEG	C	1106	7/7	0.84	0.14	31,38,48,52	0
3	EDO	A	1103	4/4	0.85	0.14	38,39,39,51	0
5	GOL	C	1107	6/6	0.85	0.14	40,51,59,64	0
5	GOL	C	1108	6/6	0.85	0.16	43,47,56,56	0
3	EDO	C	1102	4/4	0.85	0.24	38,42,45,47	0
5	GOL	A	1106	6/6	0.87	0.13	34,46,48,52	0
3	EDO	C	1104	4/4	0.90	0.18	37,38,49,54	0
2	PLP	D	1102	15/16	0.95	0.10	30,38,49,51	0
2	PLP	B	1101	15/16	0.96	0.09	29,39,45,50	0
2	PLP	C	1101	15/16	0.96	0.07	16,20,28,29	0
2	PLP	A	1101	15/16	0.97	0.07	18,23,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.