



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:38 am BST

PDB ID : 6I34
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

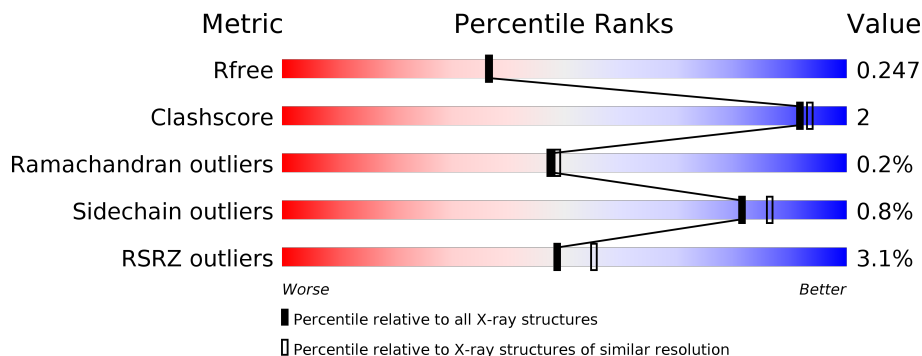
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	
1	B	984	
1	C	984	
1	D	984	

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 crite-

ria:

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](#)

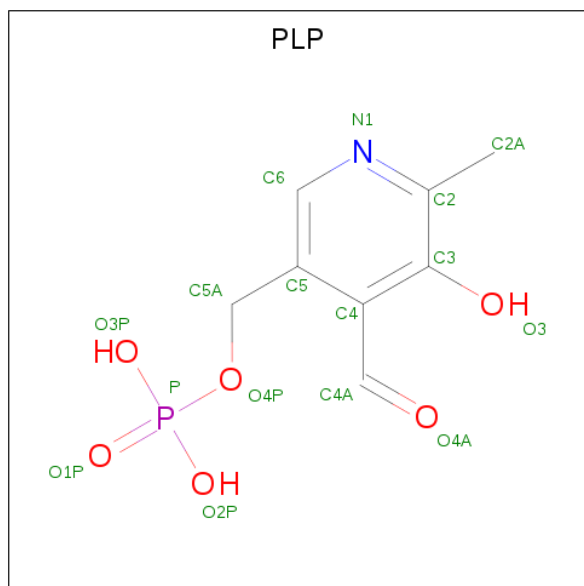
There are 6 unique types of molecules in this entry. The entry contains 31302 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



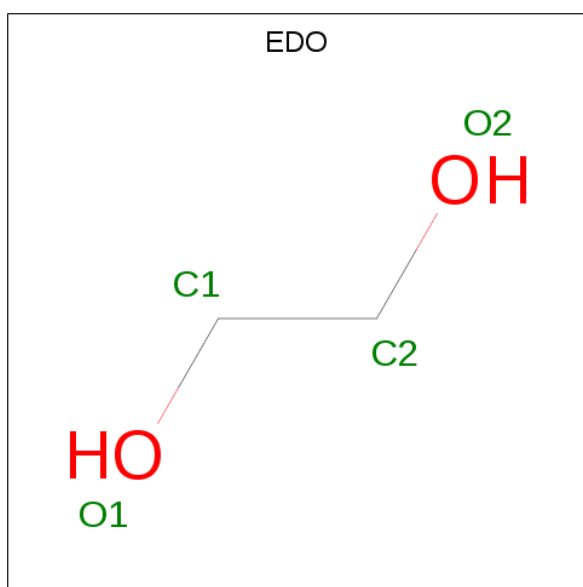
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 15	C 8	N 1	O 5	P 1	0	0
2	B	1	Total 15	C 8	N 1	O 5	P 1	0	0

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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 (three-letter code: EDO) (formula: C₂H₆O₂).



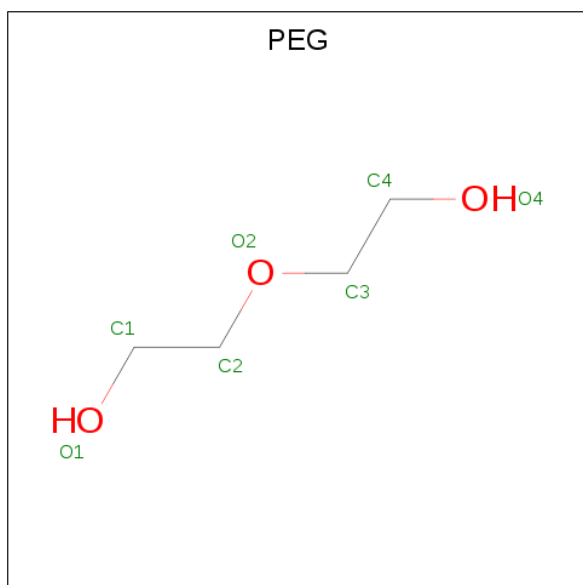
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total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

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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		

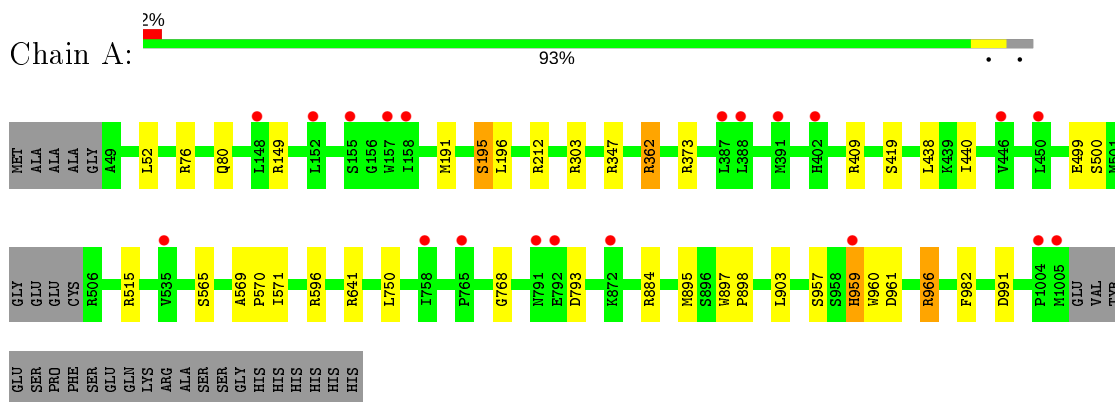
- Molecule 6 is water.

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		

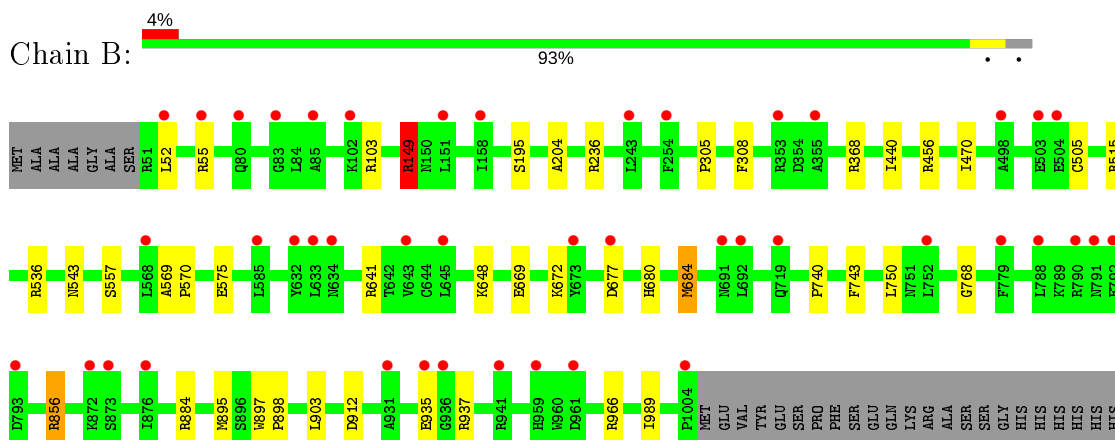
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

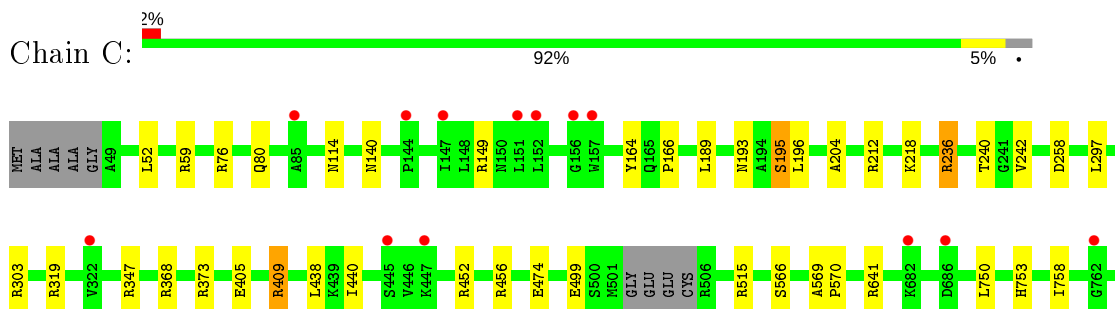
- Molecule 1: Neanderthal Glycine decarboxylase

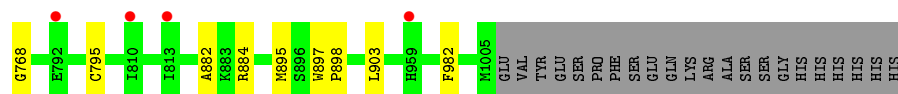


- Molecule 1: Neanderthal Glycine decarboxylase

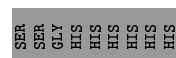
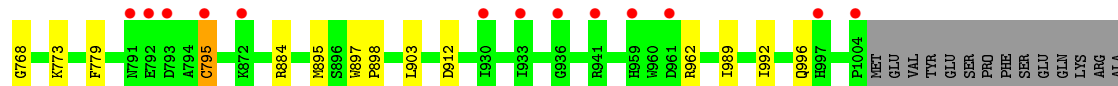
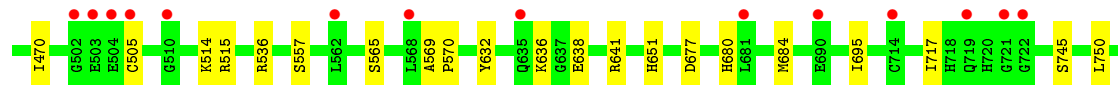
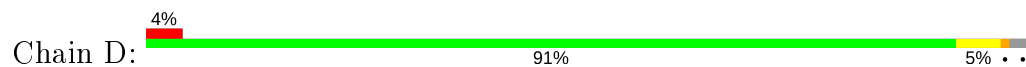


- Molecule 1: Neanderthal Glycine decarboxylase





- 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 47.85 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.90-2.10) 99.8 (47.85-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.216 , 0.243 0.223 , 0.247	Depositor DCC
R_{free} test set	12259 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: GOL, PEG, EDO, PLP

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	0.86	0/7617	0.88	13/10316 (0.1%)
1	B	0.79	1/7622 (0.0%)	0.86	14/10323 (0.1%)
1	C	0.85	2/7603 (0.0%)	0.87	14/10296 (0.1%)
1	D	0.82	1/7602 (0.0%)	0.86	15/10297 (0.1%)
All	All	0.83	4/30444 (0.0%)	0.87	56/41232 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	795	CYS	CB-SG	-7.37	1.69	1.82
1	B	575	GLU	CD-OE1	6.26	1.32	1.25
1	C	795	CYS	CB-SG	-5.22	1.73	1.81
1	C	566	SER	CB-OG	5.21	1.49	1.42

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	966	ARG	NE-CZ-NH2	10.94	125.77	120.30
1	A	966	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	D	677	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	966	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	B	149	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	212	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	D	212	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	B	966	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	A	347	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	D	236	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	149	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	C	236	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	212	ARG	NE-CZ-NH2	-6.82	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	641	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	C	347	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	641	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	149	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	195	SER	N-CA-CB	6.26	119.90	110.50
1	A	641	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	76	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	884	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	515	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	456	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	536	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	368	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	515	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	373	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	536	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	D	65	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	912	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	368	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	884	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	515	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	212	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	373	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	912	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	B	884	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	452	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	515	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	515	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	515	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	D	195	SER	N-CA-CB	5.26	118.39	110.50
1	B	677	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	212	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	195	SER	N-CA-CB	5.21	118.32	110.50
1	C	456	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	103	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	884	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	409	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	456	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	354	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	59	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	596	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	684	MET	CG-SD-CE	5.04	108.27	100.20
1	B	912	ASP	CB-CG-OD1	5.03	122.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	ASP	CB-CG-OD1	5.03	122.83	118.30

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	15	0
1	B	7454	0	7376	22	0
1	C	7436	0	7367	26	0
1	D	7434	0	7356	30	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	3	0
6	B	282	0	0	2	0
6	C	404	0	0	1	0
6	D	270	0	0	1	0
All	All	31302	0	29655	93	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 (93) 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: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:114:ASN:HB3	4:C:1106:PEG:H12	1.67	0.77
1:B:856:ARG:NH1	1:B:856:ARG:HG3	1.91	0.77
1:C:297:LEU:HD22	3:C:1102:EDO:H12	1.68	0.75
1:C:895:MET:SD	1:C:903:LEU:CD2	2.76	0.74
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: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:D:680:HIS:HE2	1:D:684:MET:HE2	1.64	0.61
1:C:474:GLU:CB	3:C:1102:EDO:H11	2.22	0.59
1:B:680:HIS:HE2	1:B:684:MET:HE2	1.67	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
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:148:LEU:C	1:D:148:LEU:HD23	2.30	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:C:882:ALA:HB2	1:C:895:MET:CE	2.41	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:684:MET:HE2	6:D:1454:HOH:O	2.12	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:895:MET:HE2	6:B:1473:HOH:O	2.13	0.48
1:B:684:MET:HE2	6:B:1467:HOH:O	2.12	0.47
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
1:A:959:HIS:NE2	1:A:961:ASP:OD2	2.50	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:HA	1:D:433:LEU:HD12	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:C:895:MET:CE	1:C:903:LEU:HD21	2.50	0.42
1:C:140:ASN:O	3:C:1102:EDO:H22	2.19	0.42
1:D:996:GLN:HB3	1:D:996:GLN:HE21	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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%)	41	41
1	B	953/984 (97%)	926 (97%)	26 (3%)	1 (0%)	51	54
1	C	949/984 (96%)	925 (98%)	23 (2%)	1 (0%)	51	54
1	D	951/984 (97%)	925 (97%)	25 (3%)	1 (0%)	51	54
All	All	3804/3936 (97%)	3699 (97%)	99 (3%)	6 (0%)	47	49

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

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Mol	Chain	Res	Type
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%)	800 (99%)	7 (1%)	78	84
1	B	807/829 (97%)	800 (99%)	7 (1%)	78	84
1	C	805/829 (97%)	800 (99%)	5 (1%)	86	90
1	D	805/829 (97%)	799 (99%)	6 (1%)	84	88
All	All	3224/3316 (97%)	3199 (99%)	25 (1%)	81	86

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

Mol	Chain	Res	Type
1	A	52	LEU
1	A	191	MET
1	A	303	ARG
1	A	362	ARG
1	A	419	SER
1	A	500	SER
1	A	571	ILE
1	B	103	ARG
1	B	149	ARG
1	B	505	CYS
1	B	557	SER
1	B	672	LYS
1	B	856	ARG
1	B	989	ILE
1	C	52	LEU
1	C	80	GLN
1	C	189	LEU
1	C	303	ARG
1	C	409	ARG

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Mol	Chain	Res	Type
1	D	103	ARG
1	D	149	ARG
1	D	505	CYS
1	D	514	LYS
1	D	557	SER
1	D	962	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	$\# Z > 2$
5	GOL	D	1105	-	5,5,5	0.53	0	5,5,5	0.44	0
3	EDO	A	1103	-	3,3,3	0.55	0	2,2,2	0.37	0
3	EDO	A	1102	-	3,3,3	0.78	0	2,2,2	0.34	0
4	PEG	B	1105	-	6,6,6	0.68	0	5,5,5	0.72	0
3	EDO	D	1104	-	3,3,3	0.65	0	2,2,2	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	C	1102	-	3,3,3	0.51	0	2,2,2	0.73	0
2	PLP	D	1102	1	15,15,16	3.49	3 (20%)	20,22,23	2.03	6 (30%)
4	PEG	A	1105	-	6,6,6	0.54	0	5,5,5	0.57	0
2	PLP	C	1101	1	15,15,16	2.93	3 (20%)	20,22,23	2.28	5 (25%)
5	GOL	C	1108	-	5,5,5	0.85	0	5,5,5	1.18	0
2	PLP	A	1101	1	15,15,16	2.43	3 (20%)	20,22,23	2.13	4 (20%)
3	EDO	C	1103	-	3,3,3	0.62	0	2,2,2	0.43	0
2	PLP	B	1101	1	15,15,16	3.42	3 (20%)	20,22,23	1.93	5 (25%)
3	EDO	C	1104	-	3,3,3	0.87	0	2,2,2	0.60	0
3	EDO	A	1104	-	3,3,3	0.39	0	2,2,2	0.52	0
5	GOL	C	1107	-	5,5,5	0.30	0	5,5,5	0.31	0
5	GOL	A	1107	-	5,5,5	0.24	0	5,5,5	0.70	0
3	EDO	B	1104	-	3,3,3	0.36	0	2,2,2	0.54	0
4	PEG	C	1106	-	6,6,6	0.53	0	5,5,5	0.70	0
4	PEG	C	1105	-	6,6,6	0.57	0	5,5,5	1.38	0
4	PEG	D	1101	-	6,6,6	0.74	0	5,5,5	0.89	0
3	EDO	B	1102	-	3,3,3	0.53	0	2,2,2	0.27	0
3	EDO	D	1103	-	3,3,3	0.92	0	2,2,2	1.07	0
3	EDO	B	1103	-	3,3,3	0.36	0	2,2,2	0.79	0
5	GOL	A	1106	-	5,5,5	0.61	0	5,5,5	0.94	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	GOL	D	1105	-	-	4/4/4/4	-
3	EDO	A	1103	-	-	1/1/1/1	-
3	EDO	A	1102	-	-	1/1/1/1	-
4	PEG	B	1105	-	-	2/4/4/4	-
3	EDO	D	1104	-	-	0/1/1/1	-
3	EDO	C	1102	-	-	0/1/1/1	-
2	PLP	D	1102	1	-	0/6/6/8	0/1/1/1
4	PEG	A	1105	-	-	1/4/4/4	-
2	PLP	C	1101	1	-	4/6/6/8	0/1/1/1
5	GOL	C	1108	-	-	4/4/4/4	-
2	PLP	A	1101	1	-	2/6/6/8	0/1/1/1
3	EDO	C	1103	-	-	0/1/1/1	-
2	PLP	B	1101	1	-	0/6/6/8	0/1/1/1
3	EDO	C	1104	-	-	1/1/1/1	-

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	PLP	C3-C2	8.92	1.49	1.40
2	C	1101	PLP	C3-C2	8.81	1.49	1.40
2	D	1102	PLP	C3-C2	8.66	1.49	1.40
2	B	1101	PLP	C5-C4	8.41	1.49	1.40
2	D	1102	PLP	C5-C4	8.39	1.49	1.40
2	A	1101	PLP	C3-C2	6.29	1.47	1.40
2	A	1101	PLP	C5-C4	5.74	1.46	1.40
2	C	1101	PLP	C5-C4	5.53	1.46	1.40
2	D	1102	PLP	C3-C4	5.28	1.51	1.40
2	B	1101	PLP	C3-C4	4.27	1.49	1.40
2	A	1101	PLP	C3-C4	2.64	1.45	1.40
2	C	1101	PLP	C3-C4	2.45	1.45	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	PLP	O4P-C5A-C5	5.90	120.60	109.35
2	C	1101	PLP	O2P-P-O4P	5.49	121.35	106.73
2	C	1101	PLP	O4P-C5A-C5	5.32	119.49	109.35
2	A	1101	PLP	O4P-P-O1P	4.59	119.36	106.47
2	D	1102	PLP	O3P-P-O4P	-4.35	95.16	106.73
2	D	1102	PLP	O4P-C5A-C5	4.07	117.10	109.35
2	D	1102	PLP	O3P-P-O2P	3.99	122.88	107.64
2	B	1101	PLP	O4P-C5A-C5	3.92	116.81	109.35
2	B	1101	PLP	O4P-P-O1P	-3.86	95.64	106.47
2	C	1101	PLP	O3P-P-O4P	-3.13	98.40	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	PLP	C3-C4-C5	-3.10	115.39	118.74
2	B	1101	PLP	C4A-C4-C5	2.90	123.93	120.94
2	A	1101	PLP	O2P-P-O4P	-2.81	99.25	106.73
2	B	1101	PLP	C6-N1-C2	2.81	124.36	119.17
2	D	1102	PLP	C6-N1-C2	2.49	123.77	119.17
2	D	1102	PLP	C3-C4-C5	-2.45	116.10	118.74
2	C	1101	PLP	C4A-C4-C5	2.29	123.29	120.94
2	A	1101	PLP	O3P-P-O4P	-2.27	100.70	106.73
2	D	1102	PLP	O4P-P-O1P	2.10	112.37	106.47
2	B	1101	PLP	O3P-P-O1P	2.01	118.54	110.68

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	1105	GOL	O1-C1-C2-C3
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
2	A	1101	PLP	C4-C5-C5A-O4P
2	A	1101	PLP	C6-C5-C5A-O4P
4	C	1105	PEG	C4-C3-O2-C2
4	C	1106	PEG	O1-C1-C2-O2
4	B	1105	PEG	O1-C1-C2-O2
4	C	1105	PEG	O1-C1-C2-O2
4	C	1105	PEG	O2-C3-C4-O4
5	D	1105	GOL	C1-C2-C3-O3
5	A	1107	GOL	C1-C2-C3-O3
5	A	1106	GOL	O1-C1-C2-C3
5	D	1105	GOL	O1-C1-C2-O2
5	C	1108	GOL	O1-C1-C2-O2
5	C	1108	GOL	O2-C2-C3-O3
5	A	1107	GOL	O2-C2-C3-O3
5	A	1106	GOL	O1-C1-C2-O2
4	A	1105	PEG	O1-C1-C2-O2
3	A	1102	EDO	O1-C1-C2-O2
3	C	1104	EDO	O1-C1-C2-O2
3	B	1102	EDO	O1-C1-C2-O2
4	C	1106	PEG	O2-C3-C4-O4
3	A	1104	EDO	O1-C1-C2-O2

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

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1105	GOL	1	0
4	B	1105	PEG	1	0
3	C	1102	EDO	5	0
4	A	1105	PEG	5	0
4	C	1106	PEG	4	0
4	C	1105	PEG	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	953/984 (96%)	0.02	20 (2%) 63 68	16, 29, 49, 81	0
1	B	954/984 (96%)	0.24	44 (4%) 32 38	21, 41, 67, 99	0
1	C	953/984 (96%)	0.04	17 (1%) 68 72	18, 29, 51, 97	0
1	D	953/984 (96%)	0.21	37 (3%) 39 45	21, 40, 64, 90	0
All	All	3813/3936 (96%)	0.13	118 (3%) 49 55	16, 34, 61, 99	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	6.9
1	C	792	GLU	5.9
1	A	959	HIS	4.1
1	B	102	LYS	4.0
1	B	55	ARG	4.0
1	C	959	HIS	3.9
1	D	1004	PRO	3.8
1	A	791	ASN	3.8
1	D	959	HIS	3.6
1	B	504	GLU	3.6
1	D	721	GLY	3.6
1	D	52	LEU	3.5
1	C	151	LEU	3.5
1	C	147	ILE	3.3
1	D	218	LYS	3.3
1	D	791	ASN	3.3
1	C	85	ALA	3.2
1	D	941	ARG	3.2
1	D	254	PHE	3.1
1	D	961	ASP	3.1
1	A	535	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	633	LEU	3.1
1	C	447	LYS	3.0
1	B	80	GLN	3.0
1	D	722	GLY	3.0
1	B	791	ASN	3.0
1	D	795	CYS	2.9
1	C	810	ILE	2.9
1	D	84	LEU	2.9
1	D	568	LEU	2.9
1	D	690	GLU	2.9
1	D	102	LYS	2.9
1	B	719	GLN	2.8
1	D	872	LYS	2.8
1	D	426	GLY	2.8
1	A	148	LEU	2.8
1	A	152	LEU	2.8
1	C	762	GLY	2.7
1	A	402	HIS	2.7
1	D	562	LEU	2.7
1	A	388	LEU	2.6
1	C	682	LYS	2.6
1	D	55	ARG	2.6
1	B	632	TYR	2.6
1	D	503	GLU	2.6
1	B	568	LEU	2.6
1	B	645	LEU	2.6
1	C	144	PRO	2.6
1	D	681	LEU	2.6
1	B	503	GLU	2.5
1	B	790	ARG	2.5
1	D	635	GLN	2.5
1	A	158	ILE	2.5
1	D	792	GLU	2.5
1	C	156	GLY	2.5
1	D	285	GLN	2.5
1	D	936	GLY	2.5
1	C	445	SER	2.5
1	A	450	LEU	2.4
1	D	504	GLU	2.4
1	B	353	ARG	2.4
1	A	792	GLU	2.4
1	A	872	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	355	ALA	2.4
1	B	1004	PRO	2.4
1	B	959	HIS	2.4
1	B	961	ASP	2.4
1	B	85	ALA	2.3
1	D	510	GLY	2.3
1	B	585	LEU	2.3
1	B	634	ASN	2.3
1	A	387	LEU	2.3
1	B	498	ALA	2.3
1	B	941	ARG	2.3
1	B	158	ILE	2.3
1	D	930	ILE	2.3
1	B	83	GLY	2.3
1	B	151	LEU	2.3
1	D	353	ARG	2.3
1	B	643	VAL	2.3
1	C	322	VAL	2.3
1	D	793	ASP	2.2
1	D	997	HIS	2.2
1	B	691	ASN	2.2
1	A	391	MET	2.2
1	B	793	ASP	2.2
1	B	254	PHE	2.2
1	B	872	LYS	2.2
1	A	758	ILE	2.2
1	D	933	ILE	2.2
1	B	673	TYR	2.2
1	B	936	GLY	2.2
1	D	719	GLN	2.2
1	C	157	TRP	2.2
1	A	155	SER	2.2
1	B	692	LEU	2.2
1	B	752	LEU	2.2
1	B	935	GLU	2.1
1	B	677	ASP	2.1
1	C	152	LEU	2.1
1	B	876	ILE	2.1
1	B	243	LEU	2.1
1	A	446	VAL	2.1
1	A	765	PRO	2.1
1	B	931	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	779	PHE	2.1
1	A	157	TRP	2.1
1	B	873	SER	2.0
1	B	788	LEU	2.0
1	C	686	ASP	2.0
1	B	792	GLU	2.0
1	D	502	GLY	2.0
1	A	1004	PRO	2.0
1	A	1005	MET	2.0
1	C	813	ILE	2.0
1	D	714	CYS	2.0
1	D	448	GLU	2.0
1	D	505	CYS	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 carbohydrates 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(\AA^2)	Q<0.9
4	PEG	A	1105	7/7	0.67	0.26	37,51,54,64	0
4	PEG	D	1101	7/7	0.71	0.26	38,41,63,65	0
3	EDO	D	1103	4/4	0.72	0.26	38,41,42,56	0
4	PEG	C	1105	7/7	0.73	0.24	37,43,48,53	0
5	GOL	C	1108	6/6	0.77	0.33	43,47,56,56	0
3	EDO	B	1103	4/4	0.77	0.27	44,50,50,53	0
4	PEG	B	1105	7/7	0.78	0.23	36,39,45,49	0
3	EDO	D	1104	4/4	0.81	0.39	33,37,46,50	0
3	EDO	C	1104	4/4	0.82	0.24	37,38,49,54	0
3	EDO	A	1102	4/4	0.83	0.25	35,35,41,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	EDO	C	1103	4/4	0.84	0.14	36,41,48,51	0
3	EDO	C	1102	4/4	0.84	0.26	38,42,45,47	0
3	EDO	B	1104	4/4	0.85	0.14	51,53,54,56	0
5	GOL	C	1107	6/6	0.86	0.15	40,51,59,64	0
5	GOL	D	1105	6/6	0.87	0.21	47,60,62,70	0
5	GOL	A	1106	6/6	0.87	0.27	34,46,48,52	0
3	EDO	B	1102	4/4	0.88	0.35	35,44,45,48	0
3	EDO	A	1104	4/4	0.89	0.18	52,55,62,66	0
5	GOL	A	1107	6/6	0.90	0.18	40,51,52,56	0
4	PEG	C	1106	7/7	0.91	0.15	31,38,48,52	0
3	EDO	A	1103	4/4	0.92	0.12	38,39,39,51	0
2	PLP	D	1102	15/16	0.96	0.17	30,38,49,51	0
2	PLP	C	1101	15/16	0.97	0.17	16,20,28,29	0
2	PLP	B	1101	15/16	0.97	0.13	29,39,45,50	0
2	PLP	A	1101	15/16	0.98	0.18	18,23,30,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.