



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:43 PM UTC

PDB ID : 5CEY / pdb_00005cey
Title : Crystal Structure of Fab 9H+3L, a putative precursor of the PGT121 family of potent HIV-1 antibodies
Authors : Wilson, I.A.; Garces, F.
Deposited on : 2015-07-07
Resolution : 2.39 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

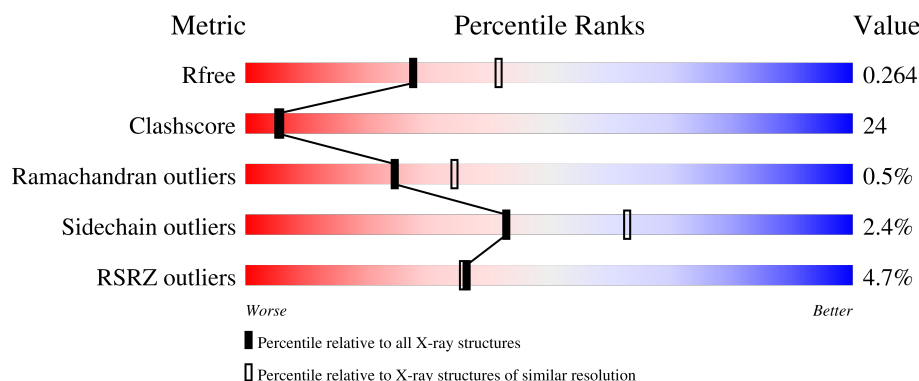
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	218	2% 68% 28% ..
1	C	218	5% 64% 26% 5%
2	B	236	5% 64% 30% 5%
2	D	236	6% 53% 34% 9% 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
4	P6G	B	301	-	-	X	-
5	PE7	D	301	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6805 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.

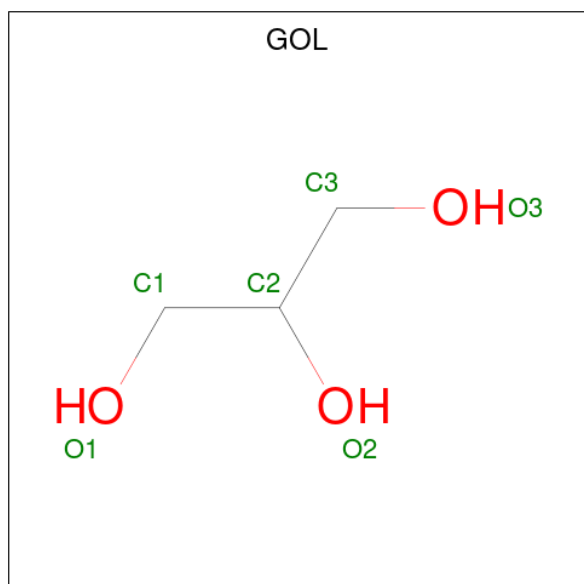
- Molecule 1 is a protein called Antibody 9H+3L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1602	1007	276	314	5			
1	C	207	Total	C	N	O	S	0	0	0
			1575	989	272	309	5			

- Molecule 2 is a protein called Antibody 9H+3L Fab heavy chain.

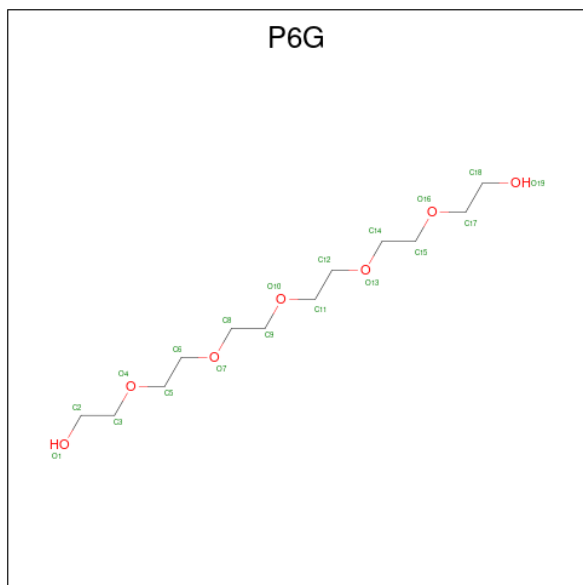
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	232	Total	C	N	O	S	0	0	0
			1760	1119	291	345	5			
2	D	225	Total	C	N	O	S	0	0	0
			1713	1093	282	333	5			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



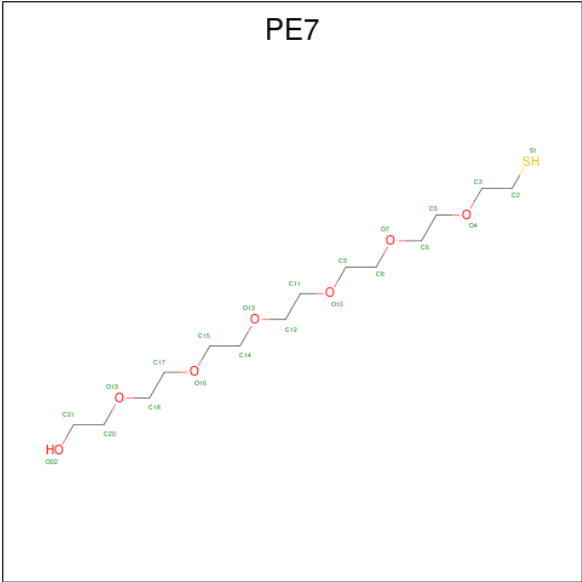
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is 1-DEOXY-1-THIO-HEPTAETHYLENE GLYCOL (CCD ID: PE7) (formula: $C_{14}H_{30}O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			22	14	7	1		

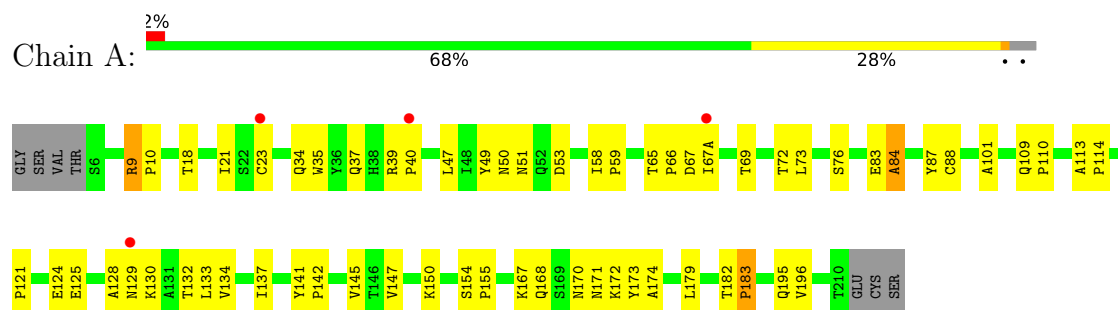
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	29	Total	O	0	0
			29	29		
6	B	25	Total	O	0	0
			25	25		
6	C	29	Total	O	0	0
			29	29		
6	D	19	Total	O	0	0
			19	19		

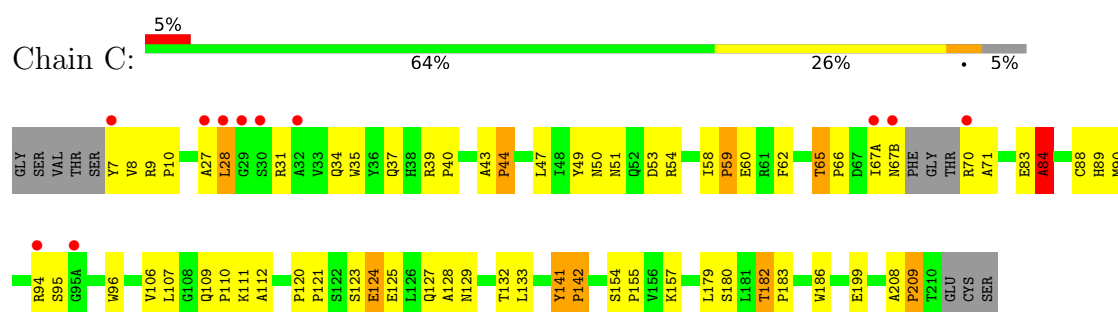
3 Residue-property plots [i](#)

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.

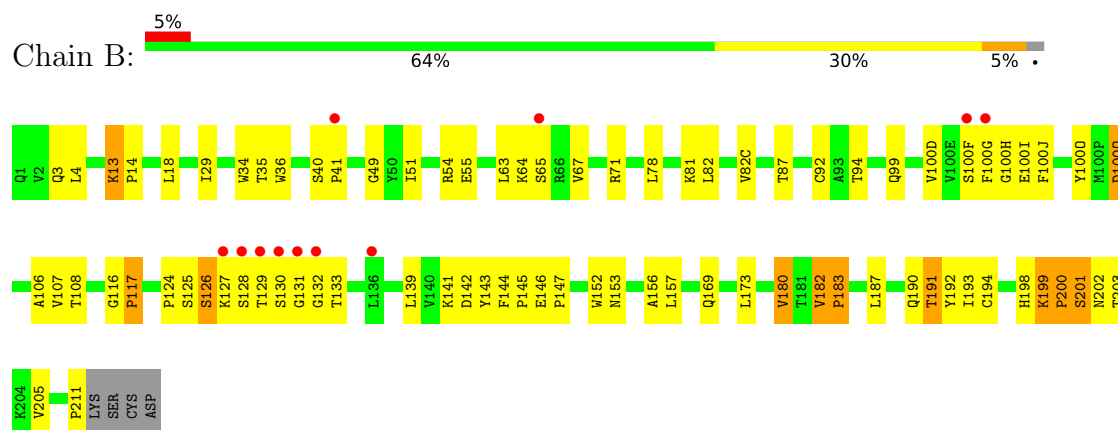
- Molecule 1: Antibody 9H+3L Fab light chain



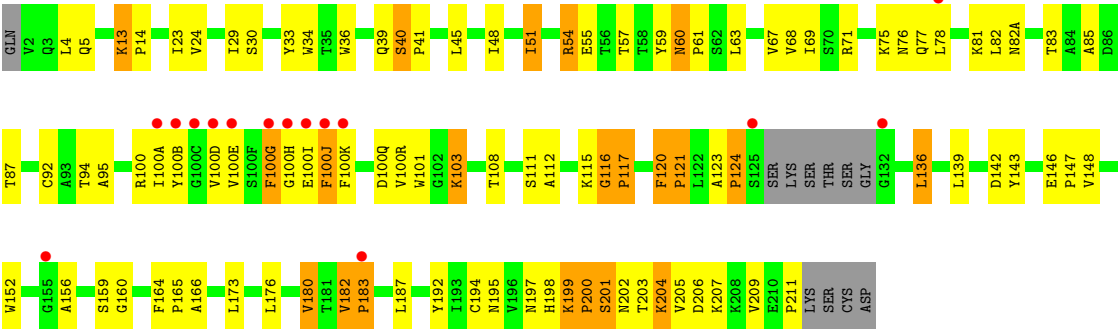
- Molecule 1: Antibody 9H+3L Fab light chain



- Molecule 2: Antibody 9H+3L Fab heavy chain



- Molecule 2: Antibody 9H+3L Fab heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.74Å 338.15Å 62.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.75 – 2.39 45.75 – 2.39	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.75-2.39) 93.2 (45.75-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.92 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.224 , 0.273 0.237 , 0.264	Depositor DCC
R_{free} test set	1646 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	1.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6805	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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: P6G, PE7, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.74	12/1645 (0.7%)	0.98	12/2245 (0.5%)
1	C	0.99	23/1616 (1.4%)	1.17	26/2205 (1.2%)
2	B	0.68	9/1804 (0.5%)	1.00	10/2462 (0.4%)
2	D	0.90	20/1756 (1.1%)	1.15	25/2397 (1.0%)
All	All	0.83	64/6821 (0.9%)	1.08	73/9309 (0.8%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	ALA	C-O	-7.67	1.14	1.24
2	B	116	GLY	C-N	6.35	1.41	1.33
1	C	110	PRO	N-CD	6.26	1.56	1.47
2	D	117	PRO	N-CD	-6.25	1.39	1.47
2	D	116	GLY	C-N	6.07	1.40	1.33
2	D	123	ALA	C-N	6.04	1.40	1.33
1	A	58	ILE	C-N	5.89	1.40	1.33
1	C	54	ARG	C-N	5.88	1.40	1.33
1	C	58	ILE	C-N	5.79	1.40	1.33
2	B	182	VAL	C-N	5.77	1.41	1.33
1	A	9	ARG	C-N	5.75	1.41	1.33
1	C	9	ARG	C-N	5.75	1.41	1.33
1	C	109	GLN	C-N	5.70	1.40	1.33
1	A	65	THR	C-N	5.68	1.41	1.33
1	C	208	ALA	C-N	5.66	1.41	1.33
1	C	142	PRO	N-CD	5.65	1.55	1.47
1	A	113	ALA	C-N	5.63	1.40	1.33
1	A	154	SER	C-N	5.63	1.40	1.33
2	D	120	PHE	C-N	5.60	1.40	1.33
2	B	13	LYS	C-N	5.60	1.40	1.33
1	C	65	THR	C-N	5.58	1.40	1.33
2	D	182	VAL	C-N	5.58	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	SER	C-N	5.56	1.40	1.33
1	C	39	ARG	C-N	5.56	1.40	1.33
2	D	40	SER	C-N	5.56	1.40	1.33
1	C	43	ALA	C-N	5.53	1.40	1.33
2	D	13	LYS	C-N	5.53	1.40	1.33
1	C	120	PRO	C-N	5.46	1.40	1.33
2	D	121	PRO	N-CD	5.38	1.55	1.47
1	A	66	PRO	N-CD	5.35	1.55	1.47
2	D	124	PRO	N-CD	5.34	1.55	1.47
1	C	183	PRO	N-CD	5.34	1.55	1.47
1	A	114	PRO	N-CD	5.33	1.55	1.47
2	B	117	PRO	N-CD	5.33	1.55	1.47
2	D	61	PRO	N-CD	5.32	1.55	1.47
1	A	155	PRO	N-CD	5.32	1.55	1.47
1	A	10	PRO	N-CD	5.31	1.55	1.47
2	D	200	PRO	N-CD	5.30	1.55	1.47
1	A	110	PRO	N-CD	5.30	1.55	1.47
2	D	41	PRO	N-CD	5.30	1.55	1.47
1	A	183	PRO	N-CD	5.29	1.55	1.47
1	C	155	PRO	N-CD	5.28	1.55	1.47
2	D	164	PHE	C-N	5.26	1.40	1.33
1	C	182	THR	C-N	5.26	1.40	1.33
2	B	41	PRO	N-CD	5.25	1.55	1.47
2	D	60	ASN	C-N	5.24	1.40	1.33
1	C	121	PRO	N-CD	5.20	1.55	1.47
1	A	59	PRO	N-CD	5.18	1.55	1.47
2	D	183	PRO	N-CD	5.18	1.55	1.47
1	C	40	PRO	N-CD	5.16	1.54	1.47
2	D	165	PRO	N-CD	5.15	1.54	1.47
2	B	200	PRO	N-CD	5.13	1.54	1.47
1	C	10	PRO	N-CD	5.12	1.54	1.47
2	B	183	PRO	N-CD	5.12	1.54	1.47
1	C	66	PRO	N-CD	5.11	1.54	1.47
1	C	44	PRO	N-CD	5.10	1.54	1.47
2	D	199	LYS	C-N	5.07	1.40	1.33
1	C	209	PRO	N-CD	5.06	1.54	1.47
2	B	40	SER	C-N	5.06	1.40	1.34
2	D	211	PRO	N-CD	5.06	1.54	1.47
1	C	59	PRO	N-CD	5.04	1.54	1.47
2	B	14	PRO	N-CD	5.02	1.54	1.47
2	D	14	PRO	N-CD	5.01	1.54	1.47
2	D	147	PRO	N-CD	5.00	1.54	1.47

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201	SER	N-CA-C	8.71	120.77	111.28
2	D	146	GLU	C-N-CD	8.49	139.27	120.60
2	B	201	SER	N-CA-C	8.04	120.05	111.28
1	C	141	TYR	C-N-CD	7.84	137.84	120.60
2	D	123	ALA	CA-C-N	-7.21	113.24	120.31
2	D	123	ALA	C-N-CA	-7.21	113.24	120.31
2	D	100(G)	PHE	N-CA-C	-7.17	103.39	111.14
2	D	116	GLY	CA-C-N	-6.94	113.50	120.31
2	D	116	GLY	C-N-CA	-6.94	113.50	120.31
2	B	116	GLY	CA-C-N	-6.90	113.55	120.31
2	B	116	GLY	C-N-CA	-6.90	113.55	120.31
1	C	54	ARG	CA-C-N	-6.83	113.27	120.03
1	C	54	ARG	C-N-CA	-6.83	113.27	120.03
1	A	58	ILE	CA-C-N	-6.70	113.40	120.03
1	A	58	ILE	C-N-CA	-6.70	113.40	120.03
2	D	182	VAL	CA-C-N	-6.68	113.10	119.85
2	D	182	VAL	C-N-CA	-6.68	113.10	119.85
2	D	48	ILE	N-CA-C	6.66	117.45	110.72
1	A	9	ARG	CA-C-N	-6.61	113.17	119.85
1	A	9	ARG	C-N-CA	-6.61	113.17	119.85
1	C	65	THR	CA-C-N	-6.53	113.25	119.85
1	C	65	THR	C-N-CA	-6.53	113.25	119.85
1	A	65	THR	CA-C-N	-6.53	113.25	119.85
1	A	65	THR	C-N-CA	-6.53	113.25	119.85
1	C	58	ILE	CA-C-N	-6.51	113.58	120.03
1	C	58	ILE	C-N-CA	-6.51	113.58	120.03
2	D	40	SER	CA-C-N	-6.49	113.08	119.76
2	D	40	SER	C-N-CA	-6.49	113.08	119.76
1	C	39	ARG	CA-C-N	-6.46	113.11	119.76
1	C	39	ARG	C-N-CA	-6.46	113.11	119.76
1	A	113	ALA	CA-C-N	-6.43	113.36	119.85
1	A	113	ALA	C-N-CA	-6.43	113.36	119.85
2	D	120	PHE	CA-C-N	-6.42	113.36	119.85
2	D	120	PHE	C-N-CA	-6.42	113.36	119.85
1	C	120	PRO	CA-C-N	-6.35	113.22	119.76
1	C	120	PRO	C-N-CA	-6.35	113.22	119.76
2	B	13	LYS	CA-C-N	-6.35	113.22	119.76
2	B	13	LYS	C-N-CA	-6.35	113.22	119.76
1	C	208	ALA	CA-C-N	-6.33	113.24	119.76
1	C	208	ALA	C-N-CA	-6.33	113.24	119.76
1	C	43	ALA	CA-C-N	-6.33	113.46	119.85
1	C	43	ALA	C-N-CA	-6.33	113.46	119.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	GLN	CA-C-N	-6.30	114.14	120.31
1	C	109	GLN	C-N-CA	-6.30	114.14	120.31
2	D	164	PHE	CA-C-N	-6.27	113.32	119.78
2	D	164	PHE	C-N-CA	-6.27	113.32	119.78
1	C	154	SER	CA-C-N	-6.26	113.52	119.85
1	C	154	SER	C-N-CA	-6.26	113.52	119.85
2	B	182	VAL	CA-C-N	-6.26	113.53	119.85
2	B	182	VAL	C-N-CA	-6.26	113.53	119.85
2	D	13	LYS	CA-C-N	-6.13	113.45	119.76
2	D	13	LYS	C-N-CA	-6.13	113.45	119.76
2	D	147	PRO	CA-N-CD	-6.13	102.92	111.50
1	A	154	SER	CA-C-N	-6.09	113.70	119.85
1	A	154	SER	C-N-CA	-6.09	113.70	119.85
1	C	9	ARG	CA-C-N	-6.05	113.46	119.99
1	C	9	ARG	C-N-CA	-6.05	113.46	119.99
1	C	95	SER	N-CA-C	5.68	120.21	113.28
1	C	28	LEU	N-CA-C	5.65	117.52	111.36
2	B	40	SER	CA-C-N	-5.57	112.87	119.05
2	B	40	SER	C-N-CA	-5.57	112.87	119.05
2	D	199	LYS	CA-C-N	-5.46	113.27	119.28
2	D	199	LYS	C-N-CA	-5.46	113.27	119.28
2	B	100(Q)	ASP	N-CA-C	5.41	117.25	111.36
1	C	84	ALA	CB-CA-C	-5.30	99.87	110.42
1	C	182	THR	CA-C-N	-5.24	113.52	119.28
1	C	182	THR	C-N-CA	-5.24	113.52	119.28
2	D	100(Q)	ASP	N-CA-C	5.24	117.07	111.36
1	A	182	THR	CA-C-N	-5.22	113.26	119.05
1	A	182	THR	C-N-CA	-5.22	113.26	119.05
2	D	156	ALA	N-CA-C	5.21	116.96	111.28
2	D	60	ASN	CA-C-N	-5.16	113.60	119.28
2	D	60	ASN	C-N-CA	-5.16	113.60	119.28

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	1602	0	1548	50	0
1	C	1575	0	1521	49	0
2	B	1760	0	1740	109	0
2	D	1713	0	1690	122	0
3	A	6	0	8	1	0
3	C	6	0	8	0	0
4	B	19	0	26	11	0
5	D	22	0	30	18	0
6	A	29	0	0	1	0
6	B	25	0	0	4	0
6	C	29	0	0	0	0
6	D	19	0	0	1	0
All	All	6805	0	6571	318	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 24.

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:GLU:CG	2:B:71:ARG:HH21	1.23	1.45
1:A:23:CYS:SG	1:A:88:CYS:SG	1.46	1.38
1:A:23:CYS:CB	1:A:88:CYS:SG	2.18	1.31
2:B:55:GLU:HG3	2:B:71:ARG:NH2	1.50	1.24
2:B:55:GLU:CG	2:B:71:ARG:NH2	2.05	1.17
2:B:55:GLU:HG2	2:B:71:ARG:HH21	1.06	1.16
2:B:55:GLU:HG3	2:B:71:ARG:HH21	1.00	1.15
2:B:29:ILE:HD11	2:B:78:LEU:CD2	1.79	1.13
2:D:136:LEU:HD22	2:D:180:VAL:HG13	1.29	1.11
2:B:81:LYS:HZ3	4:B:301:P6G:H81	1.12	1.10
2:D:55:GLU:HG3	2:D:71:ARG:NH2	1.66	1.10
1:A:142:PRO:HB2	3:A:301:GOL:H12	1.36	1.07
2:D:100(D):VAL:CG1	2:D:100(G):PHE:HD1	1.65	1.07
2:D:100(D):VAL:CG1	2:D:100(G):PHE:CD1	2.40	1.05
2:D:100(E):VAL:HA	2:D:100(H):GLY:HA2	1.34	1.05
2:B:81:LYS:NZ	4:B:301:P6G:H81	1.73	1.03
2:D:55:GLU:CG	2:D:71:ARG:HH21	1.71	1.02
2:D:136:LEU:HD22	2:D:180:VAL:CG1	1.91	1.00
1:A:23:CYS:HB3	1:A:88:CYS:SG	2.02	0.97
2:B:34:TRP:CD2	2:B:78:LEU:HD11	2.00	0.97
2:B:13:LYS:NZ	1:C:182:THR:HG22	1.79	0.96
2:D:100(B):TYR:OH	2:D:100(I):GLU:HB3	1.66	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:N	1:A:124:GLU:OE1	1.98	0.96
2:D:55:GLU:HG3	2:D:71:ARG:HH21	0.80	0.95
1:C:28:LEU:HD12	1:C:94:ARG:HD2	1.48	0.95
2:D:100(E):VAL:O	2:D:100(H):GLY:HA3	1.67	0.94
2:D:136:LEU:CD2	2:D:180:VAL:CG1	2.46	0.94
2:B:29:ILE:HD11	2:B:78:LEU:HD21	1.50	0.93
2:D:209:VAL:O	6:D:401:HOH:O	1.87	0.93
2:D:100(D):VAL:HG11	2:D:100(G):PHE:CD1	2.03	0.93
1:C:111:LYS:HD2	1:C:199:GLU:HG3	1.53	0.91
2:D:100(E):VAL:HA	2:D:100(H):GLY:CA	2.00	0.91
2:B:29:ILE:HD11	2:B:78:LEU:HD23	1.51	0.90
2:B:34:TRP:CG	2:B:78:LEU:HD11	2.07	0.89
2:B:130:SER:OG	6:B:401:HOH:O	1.88	0.89
2:D:13:LYS:NZ	2:D:111:SER:O	2.05	0.88
2:B:100(D):VAL:HG12	2:B:100(I):GLU:OE1	1.74	0.88
2:B:117:PRO:HB3	2:B:143:TYR:HB3	1.56	0.87
2:D:81:LYS:HZ3	5:D:301:PE7:H141	1.40	0.87
1:A:167:LYS:HE2	1:A:173:TYR:CE1	2.09	0.87
2:B:132:GLY:O	2:B:183:PRO:HA	1.74	0.87
1:A:125:GLU:OE1	6:A:401:HOH:O	1.92	0.86
1:A:23:CYS:SG	1:A:88:CYS:CB	2.63	0.86
2:D:100(D):VAL:HG13	2:D:100(G):PHE:HD1	1.41	0.85
2:D:142:ASP:HB3	2:D:173:LEU:HD13	1.58	0.84
2:B:129:THR:O	2:B:130:SER:OG	1.97	0.82
2:D:100(D):VAL:O	2:D:100(H):GLY:N	2.11	0.82
2:B:201:SER:OG	2:B:203:THR:N	2.13	0.81
2:B:100(D):VAL:HG11	2:B:100(G):PHE:CD2	2.15	0.81
1:C:124:GLU:HG3	2:D:121:PRO:HD2	1.61	0.81
2:D:81:LYS:HE2	5:D:301:PE7:H111	1.63	0.80
2:B:55:GLU:HG2	2:B:71:ARG:NH2	1.86	0.80
2:B:127:LYS:HB3	2:B:128:SER:HB3	1.62	0.80
2:D:81:LYS:HE3	5:D:301:PE7:H32	1.63	0.80
2:D:197:ASN:ND2	2:D:204:LYS:HE3	1.97	0.79
2:D:100(E):VAL:CA	2:D:100(H):GLY:HA2	2.12	0.77
2:B:198:HIS:ND1	2:B:201:SER:HB3	2.00	0.76
1:C:49:TYR:O	1:C:53:ASP:HB2	1.84	0.76
2:D:198:HIS:ND1	2:D:201:SER:OG	2.20	0.75
2:D:136:LEU:CD2	2:D:180:VAL:HG13	2.08	0.75
1:A:125:GLU:HG2	1:A:130:LYS:O	1.87	0.75
2:B:13:LYS:HZ2	1:C:182:THR:HG22	1.50	0.75
1:C:50:ASN:ND2	1:C:53:ASP:OD2	2.18	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:THR:OG1	6:B:402:HOH:O	2.03	0.74
2:B:87:THR:HG23	2:B:108:THR:HA	1.70	0.74
1:C:27:ALA:HB2	1:C:90:MET:CE	2.17	0.74
2:D:68:VAL:HG12	5:D:301:PE7:H201	1.68	0.73
2:D:100(A):ILE:HD12	2:D:100(A):ILE:N	2.03	0.73
2:B:81:LYS:HE2	4:B:301:P6G:H82	1.71	0.72
2:D:40:SER:OG	2:D:87:THR:O	2.05	0.72
2:D:136:LEU:C	2:D:136:LEU:HD23	2.14	0.72
1:C:27:ALA:HB2	1:C:90:MET:SD	2.30	0.71
2:D:100(E):VAL:CA	2:D:100(H):GLY:CA	2.69	0.71
2:B:13:LYS:HZ3	1:C:182:THR:HG22	1.54	0.70
2:B:169:GLN:NE2	6:B:404:HOH:O	2.22	0.70
1:C:28:LEU:CD1	1:C:94:ARG:HD2	2.22	0.70
1:C:111:LYS:CD	1:C:199:GLU:HG3	2.21	0.70
2:D:100(A):ILE:HG13	2:D:100(J):PHE:HB3	1.72	0.70
2:D:81:LYS:HZ3	5:D:301:PE7:H112	1.57	0.69
2:D:100(E):VAL:C	2:D:100(H):GLY:CA	2.66	0.69
2:B:29:ILE:CD1	2:B:71:ARG:HG3	2.24	0.68
2:D:100(D):VAL:HG11	2:D:100(G):PHE:HD1	1.47	0.68
2:B:34:TRP:CD2	2:B:78:LEU:CD1	2.75	0.68
2:B:100(D):VAL:HG13	2:B:100(F):SER:O	1.94	0.68
2:B:81:LYS:HE2	4:B:301:P6G:H51	1.77	0.67
1:A:167:LYS:HE2	1:A:173:TYR:CZ	2.30	0.66
2:B:34:TRP:CG	2:B:78:LEU:CD1	2.79	0.66
1:A:18:THR:HG22	1:A:76:SER:HA	1.77	0.66
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.78	0.66
2:D:30:SER:HA	2:D:71:ARG:HH11	1.60	0.66
2:D:30:SER:HA	2:D:71:ARG:NH1	2.11	0.66
1:C:125:GLU:OE2	1:C:132:THR:OG1	2.13	0.65
2:B:100(D):VAL:O	2:B:100(I):GLU:HG3	1.96	0.65
2:D:100(E):VAL:C	2:D:100(H):GLY:HA3	2.19	0.65
2:D:117:PRO:HB3	2:D:143:TYR:HB3	1.79	0.65
2:D:81:LYS:CE	5:D:301:PE7:H32	2.27	0.64
2:B:64:LYS:O	2:B:65:SER:HB3	1.96	0.64
1:A:23:CYS:SG	1:A:35:TRP:CZ2	2.91	0.63
2:D:81:LYS:NZ	5:D:301:PE7:H112	2.13	0.63
1:C:111:LYS:HD2	1:C:199:GLU:CG	2.27	0.63
2:D:182:VAL:HG11	2:D:192:TYR:OH	1.98	0.63
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.81	0.62
2:B:81:LYS:CE	4:B:301:P6G:C8	2.78	0.62
1:A:67:ASP:HA	1:A:69:THR:HB	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:CG2	1:A:196:VAL:HG13	2.30	0.62
2:D:195:ASN:ND2	2:D:206:ASP:OD1	2.22	0.62
1:A:170:ASN:O	1:A:171:ASN:HB2	2.00	0.62
2:B:100(D):VAL:HG12	2:B:100(I):GLU:CD	2.25	0.61
2:D:100:ARG:HB3	2:D:100(K):PHE:CZ	2.35	0.61
2:B:142:ASP:HB3	2:B:173:LEU:HD23	1.82	0.61
2:D:100(D):VAL:HG11	2:D:100(G):PHE:CE1	2.35	0.61
2:B:55:GLU:HG3	2:B:71:ARG:HH22	1.61	0.61
1:A:125:GLU:OE2	1:A:132:THR:HG23	2.01	0.61
2:D:136:LEU:CD2	2:D:180:VAL:HG12	2.31	0.61
2:D:100(E):VAL:O	2:D:100(H):GLY:CA	2.47	0.61
2:B:129:THR:O	2:B:129:THR:HG22	2.01	0.60
2:D:100(A):ILE:HD12	2:D:100(A):ILE:H	1.67	0.60
2:D:51:ILE:HG13	2:D:57:THR:HG22	1.84	0.60
2:B:201:SER:O	1:C:128:ALA:HB1	2.02	0.59
2:B:81:LYS:CE	4:B:301:P6G:H51	2.33	0.59
2:D:100(D):VAL:O	2:D:100(H):GLY:CA	2.50	0.59
2:B:29:ILE:HD13	2:B:71:ARG:HG3	1.84	0.58
1:C:67(A):ILE:C	1:C:67(B):ASN:HD22	2.11	0.58
2:D:81:LYS:CE	5:D:301:PE7:H82	2.32	0.58
2:B:81:LYS:HE2	4:B:301:P6G:C8	2.33	0.58
1:C:28:LEU:HD13	1:C:94:ARG:NE	2.17	0.58
2:B:81:LYS:CE	4:B:301:P6G:H82	2.34	0.58
2:B:199:LYS:O	2:B:202:ASN:HB3	2.03	0.58
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.86	0.58
2:D:94:THR:HG22	2:D:100(R):VAL:HB	1.86	0.58
1:A:145:VAL:CG2	1:A:196:VAL:CG1	2.82	0.57
2:B:81:LYS:CE	4:B:301:P6G:H81	2.33	0.57
2:B:100(D):VAL:CG1	2:B:100(G):PHE:CD2	2.86	0.57
1:C:141:TYR:CG	1:C:142:PRO:HA	2.39	0.57
2:B:100(G):PHE:CD1	2:B:100(G):PHE:N	2.72	0.56
2:D:68:VAL:HG13	2:D:81:LYS:HB2	1.87	0.56
2:D:68:VAL:CG1	2:D:81:LYS:HB2	2.36	0.56
2:D:100:ARG:NH1	2:D:100(A):ILE:O	2.38	0.56
2:B:81:LYS:NZ	4:B:301:P6G:C8	2.60	0.56
2:D:100(D):VAL:O	2:D:100(H):GLY:HA2	2.05	0.56
2:D:182:VAL:HG13	2:D:183:PRO:CD	2.36	0.56
1:A:145:VAL:HG21	1:A:196:VAL:CG1	2.36	0.56
2:B:34:TRP:HB3	2:B:78:LEU:HD13	1.87	0.55
1:C:70:ARG:HG3	1:C:70:ARG:O	2.07	0.55
2:D:68:VAL:CG1	5:D:301:PE7:H201	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:ASN:HD21	2:D:204:LYS:HE3	1.72	0.55
2:B:125:SER:O	2:B:126:SER:HB2	2.08	0.54
2:D:34:TRP:HB3	2:D:78:LEU:CD2	2.36	0.54
1:C:35:TRP:CZ3	1:C:88:CYS:HB2	2.43	0.54
2:D:82(A):ASN:CG	5:D:301:PE7:H211	2.33	0.54
2:B:100(J):PHE:CD1	2:B:100(J):PHE:C	2.86	0.54
2:D:5:GLN:HE22	2:D:103:LYS:CE	2.21	0.54
1:A:168:GLN:NE2	1:A:170:ASN:OD1	2.40	0.54
2:D:5:GLN:HE22	2:D:103:LYS:HE3	1.72	0.54
1:C:186:TRP:CE2	1:C:209:PRO:HG3	2.43	0.53
1:A:21:ILE:HD12	1:A:73:LEU:HD23	1.91	0.53
2:D:116:GLY:HA2	2:D:201:SER:OG	2.09	0.53
1:C:60:GLU:CD	1:C:60:GLU:H	2.17	0.53
2:D:34:TRP:HB3	2:D:78:LEU:HD22	1.91	0.52
2:D:59:TYR:HE1	2:D:69:ILE:HG13	1.74	0.52
2:D:67:VAL:HG22	2:D:82:LEU:CD1	2.39	0.52
2:B:201:SER:N	2:B:202:ASN:HA	2.25	0.52
2:B:124:PRO:HD2	2:B:211:PRO:HA	1.91	0.52
2:B:34:TRP:CZ3	2:B:94:THR:HG22	2.45	0.52
1:A:168:GLN:HG3	1:A:172:LYS:O	2.09	0.51
2:B:157:LEU:HD21	2:B:180:VAL:HG21	1.92	0.51
1:C:67(B):ASN:HD22	1:C:67(B):ASN:N	2.09	0.51
1:C:28:LEU:CD1	1:C:94:ARG:CD	2.87	0.51
2:D:4:LEU:HG	2:D:24:VAL:HG12	1.92	0.51
2:D:81:LYS:CE	5:D:301:PE7:H111	2.38	0.51
2:D:115:LYS:NZ	2:D:142:ASP:O	2.41	0.51
2:B:173:LEU:N	2:B:173:LEU:CD1	2.74	0.51
1:C:125:GLU:HG3	2:D:120:PHE:CE2	2.46	0.51
2:B:100(O):TYR:OH	6:B:403:HOH:O	2.19	0.51
1:C:31:ARG:NH2	1:C:71:ALA:H	2.09	0.51
1:A:21:ILE:O	1:A:72:THR:HA	2.11	0.50
1:A:34:GLN:HG3	1:A:49:TYR:HA	1.92	0.50
2:B:100(Q):ASP:OD1	2:B:100(Q):ASP:N	2.28	0.50
1:C:31:ARG:HH22	1:C:71:ALA:H	1.58	0.50
1:C:50:ASN:O	1:C:51:ASN:HB2	2.11	0.50
2:B:100(F):SER:C	2:B:100(G):PHE:CD1	2.89	0.50
2:B:203:THR:HG22	2:B:205:VAL:HG23	1.93	0.50
1:C:59:PRO:HD2	1:C:62:PHE:CD2	2.47	0.50
2:D:23:ILE:HD13	2:D:77:GLN:HB3	1.93	0.50
2:D:63:LEU:O	2:D:67:VAL:HG23	2.11	0.50
2:D:152:TRP:CH2	2:D:194:CYS:HB3	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD21	2:B:34:TRP:HZ3	1.77	0.50
1:C:106:VAL:C	1:C:107:LEU:HD23	2.36	0.50
2:B:99:GLN:HG3	2:B:99:GLN:O	2.11	0.50
1:C:44:PRO:HD2	2:D:101:TRP:CE3	2.46	0.50
2:D:100(K):PHE:C	2:D:100(K):PHE:CD1	2.90	0.49
1:A:35:TRP:CH2	1:A:88:CYS:HB2	2.47	0.49
1:C:67(A):ILE:HB	1:C:67(B):ASN:HD22	1.76	0.49
2:B:100(D):VAL:HG11	2:B:100(G):PHE:CE2	2.46	0.49
2:D:166:ALA:HB2	2:D:176:LEU:HD23	1.95	0.49
1:C:67(B):ASN:N	1:C:67(B):ASN:ND2	2.60	0.49
2:D:136:LEU:HD23	2:D:136:LEU:O	2.12	0.49
1:A:128:ALA:CB	2:D:201:SER:O	2.61	0.49
2:D:182:VAL:HG13	2:D:183:PRO:HD2	1.95	0.49
5:D:301:PE7:S1	5:D:301:PE7:H172	2.52	0.49
2:B:152:TRP:CH2	2:B:194:CYS:HB3	2.48	0.49
2:D:100(A):ILE:HG13	2:D:100(J):PHE:CB	2.42	0.49
2:B:100(F):SER:C	2:B:100(G):PHE:CG	2.92	0.48
2:B:54:ARG:O	2:B:55:GLU:HB2	2.12	0.48
2:D:67:VAL:HG22	2:D:82:LEU:HD13	1.94	0.48
2:D:83:THR:HG23	2:D:85:ALA:H	1.78	0.48
2:B:18:LEU:HD11	2:B:107:VAL:HG11	1.95	0.48
2:D:36:TRP:CZ3	2:D:92:CYS:HB3	2.49	0.47
2:D:142:ASP:HB3	2:D:173:LEU:CD1	2.38	0.47
2:D:180:VAL:HG22	2:D:182:VAL:HG23	1.96	0.47
2:B:18:LEU:HB3	2:B:82:LEU:HB3	1.96	0.47
2:B:190:GLN:OE1	2:B:191:THR:HG22	2.14	0.47
2:D:81:LYS:HZ3	5:D:301:PE7:C11	2.26	0.47
2:B:190:GLN:OE1	2:B:191:THR:N	2.37	0.47
1:A:167:LYS:HE2	1:A:173:TYR:HE1	1.76	0.47
2:B:100(D):VAL:H	2:B:100(I):GLU:HG3	1.79	0.47
1:C:50:ASN:HB3	1:C:53:ASP:OD2	2.13	0.47
2:B:13:LYS:HD2	1:C:182:THR:CG2	2.45	0.47
2:B:34:TRP:CE3	2:B:78:LEU:CD1	2.97	0.47
2:D:81:LYS:NZ	5:D:301:PE7:C11	2.78	0.47
5:D:301:PE7:S1	5:D:301:PE7:C17	3.03	0.47
2:D:182:VAL:CG1	2:D:183:PRO:CD	2.93	0.47
2:D:81:LYS:HE2	5:D:301:PE7:H82	1.95	0.46
2:B:18:LEU:HB2	2:B:82(C):VAL:HG11	1.97	0.46
1:A:132:THR:HG21	2:B:141:LYS:NZ	2.30	0.46
1:A:137:ILE:CD1	1:A:196:VAL:HG21	2.45	0.46
1:A:147:VAL:HG13	1:A:196:VAL:HG22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:THR:HA	2:B:182:VAL:O	2.16	0.46
2:D:54:ARG:O	2:D:55:GLU:HB2	2.14	0.46
2:D:87:THR:HG23	2:D:108:THR:HA	1.98	0.46
2:D:100(E):VAL:HA	2:D:100(H):GLY:HA3	1.93	0.46
1:A:129:ASN:HA	1:A:183:PRO:HG2	1.97	0.46
2:B:29:ILE:HD11	2:B:71:ARG:HG3	1.97	0.46
2:B:3:GLN:C	2:B:4:LEU:HD12	2.41	0.45
2:B:100(D):VAL:CG1	2:B:100(I):GLU:HG3	2.46	0.45
2:B:129:THR:C	2:B:130:SER:HG	2.11	0.45
2:D:198:HIS:CD2	2:D:200:PRO:HD2	2.51	0.45
2:B:173:LEU:N	2:B:173:LEU:HD12	2.31	0.45
1:C:35:TRP:CH2	1:C:88:CYS:HB2	2.50	0.45
1:C:111:LYS:HD2	1:C:199:GLU:CB	2.47	0.45
2:B:100(D):VAL:H	2:B:100(I):GLU:CG	2.28	0.45
1:A:121:PRO:HD3	1:A:133:LEU:HG	1.98	0.45
2:B:34:TRP:CB	2:B:78:LEU:HD13	2.46	0.45
2:D:136:LEU:HD23	2:D:180:VAL:HG12	1.99	0.45
2:B:144:PHE:HA	2:B:145:PRO:HA	1.75	0.45
1:C:28:LEU:HD13	1:C:94:ARG:HE	1.79	0.45
1:C:28:LEU:HD12	1:C:94:ARG:CD	2.31	0.45
1:C:179:LEU:HD12	1:C:180:SER:N	2.31	0.45
1:A:145:VAL:HG22	1:A:196:VAL:HG13	1.98	0.45
1:A:150:LYS:NZ	1:A:195:GLN:OE1	2.37	0.45
2:B:100(F):SER:O	2:B:100(G):PHE:CG	2.70	0.45
2:D:100(H):GLY:O	2:D:100(J):PHE:CE2	2.70	0.44
1:A:128:ALA:HB2	2:D:201:SER:O	2.17	0.44
2:D:100(I):GLU:O	2:D:100(J):PHE:CD1	2.70	0.44
1:C:28:LEU:CD1	1:C:94:ARG:NE	2.81	0.44
1:A:83:GLU:O	1:A:84:ALA:HB2	2.18	0.44
2:B:36:TRP:CZ3	2:B:92:CYS:HB3	2.52	0.44
2:B:198:HIS:CD2	2:B:200:PRO:HD2	2.52	0.44
1:A:67(A):ILE:H	1:A:67(A):ILE:HG13	1.49	0.44
2:D:81:LYS:CD	5:D:301:PE7:H171	2.48	0.44
1:A:129:ASN:OD1	1:A:183:PRO:HD2	2.18	0.43
2:D:199:LYS:O	2:D:202:ASN:HB3	2.18	0.43
2:B:81:LYS:NZ	4:B:301:P6G:H31	2.34	0.43
2:D:29:ILE:HG23	2:D:71:ARG:HD2	2.01	0.43
1:A:21:ILE:O	1:A:73:LEU:N	2.41	0.43
2:D:201:SER:HB2	2:D:203:THR:N	2.34	0.43
2:D:143:TYR:CE1	2:D:148:VAL:HG23	2.53	0.43
1:A:168:GLN:OE1	1:A:174:ALA:HB2	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD11	1:A:196:VAL:HG21	2.01	0.43
2:B:100(H):GLY:HA2	2:B:100(J):PHE:CE2	2.54	0.42
1:C:96:TRP:HB3	2:D:60:ASN:ND2	2.33	0.42
2:B:152:TRP:CZ3	2:B:194:CYS:HB3	2.54	0.42
2:B:190:GLN:HB3	2:B:192:TYR:CE2	2.54	0.42
1:C:34:GLN:HB2	1:C:89:HIS:HB3	2.01	0.42
2:D:100(G):PHE:CD1	2:D:100(G):PHE:N	2.87	0.42
1:A:133:LEU:HD13	1:A:179:LEU:HD23	2.01	0.42
2:D:36:TRP:CH2	2:D:92:CYS:HB3	2.54	0.42
2:D:201:SER:N	2:D:202:ASN:HA	2.34	0.42
2:B:124:PRO:HG3	2:B:187:LEU:HD22	2.01	0.42
2:D:159:SER:HA	2:D:160:GLY:HA2	1.69	0.42
1:C:133:LEU:HB2	1:C:179:LEU:HB3	2.01	0.42
2:D:100(D):VAL:HG13	2:D:100(G):PHE:CD1	2.30	0.42
2:D:205:VAL:HG12	2:D:207:LYS:HG2	2.01	0.42
1:A:49:TYR:O	1:A:53:ASP:HB2	2.19	0.42
2:D:136:LEU:CD2	2:D:136:LEU:C	2.86	0.42
1:A:109:GLN:HB2	1:A:141:TYR:CE1	2.55	0.42
2:B:100(D):VAL:HG13	2:B:100(I):GLU:HG3	2.01	0.41
2:D:33:TYR:HB2	2:D:95:ALA:O	2.19	0.41
2:B:127:LYS:HA	2:B:128:SER:HA	1.81	0.41
2:B:34:TRP:CH2	2:B:94:THR:HG22	2.56	0.41
2:B:63:LEU:O	2:B:67:VAL:HG22	2.21	0.41
1:A:167:LYS:CE	1:A:173:TYR:CE1	2.94	0.41
2:B:129:THR:C	2:B:131:GLY:H	2.26	0.41
1:C:7:TYR:O	1:C:7:TYR:CD1	2.74	0.41
2:D:82(A):ASN:HB3	5:D:301:PE7:H211	2.03	0.41
2:B:146:GLU:HA	2:B:147:PRO:HA	1.85	0.41
2:B:153:ASN:CB	2:B:156:ALA:HB3	2.51	0.41
1:A:39:ARG:HA	1:A:40:PRO:HD2	1.82	0.41
2:B:106:ALA:HB3	2:B:147:PRO:HD3	2.03	0.41
2:B:198:HIS:ND1	2:B:201:SER:CB	2.78	0.41
2:B:202:ASN:OD1	2:B:202:ASN:N	2.51	0.40
1:C:83:GLU:O	1:C:84:ALA:HB2	2.21	0.40
1:C:123:SER:O	1:C:127:GLN:HG3	2.20	0.40
2:D:124:PRO:HG3	2:D:187:LEU:HD22	2.03	0.40
1:A:50:ASN:O	1:A:51:ASN:HB2	2.21	0.40
1:A:87:TYR:CZ	1:A:101:ALA:HB2	2.57	0.40
2:D:13:LYS:NZ	2:D:112:ALA:O	2.51	0.40
2:D:166:ALA:HA	2:D:176:LEU:HB3	2.04	0.40
1:A:87:TYR:CE1	1:A:101:ALA:HB2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:VAL:HG21	2:B:139:LEU:HD13	2.03	0.40
2:B:35:THR:OG1	2:B:49:GLY:O	2.38	0.40
2:B:153:ASN:HB3	2:B:156:ALA:HB3	2.04	0.40
2:D:100(B):TYR:CZ	2:D:100(I):GLU:HB3	2.50	0.40
2:D:182:VAL:HG12	2:D:183:PRO:N	2.37	0.40
2:B:51:ILE:O	2:B:51:ILE:HG23	2.21	0.40
1:C:124:GLU:HG3	2:D:121:PRO:CD	2.43	0.40
2:D:24:VAL:HG22	2:D:76:ASN:O	2.21	0.40
2:D:100(E):VAL:C	2:D:100(H):GLY:N	2.79	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	209/218 (96%)	203 (97%)	5 (2%)	1 (0%)	24	34
1	C	203/218 (93%)	200 (98%)	2 (1%)	1 (0%)	24	34
2	B	230/236 (98%)	224 (97%)	5 (2%)	1 (0%)	30	40
2	D	221/236 (94%)	217 (98%)	3 (1%)	1 (0%)	24	34
All	All	863/908 (95%)	844 (98%)	15 (2%)	4 (0%)	24	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	84	ALA
1	A	84	ALA
2	B	126	SER
2	D	100(J)	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	175/181 (97%)	174 (99%)	1 (1%)	78	88
1	C	172/181 (95%)	167 (97%)	5 (3%)	37	57
2	B	200/204 (98%)	196 (98%)	4 (2%)	48	68
2	D	194/204 (95%)	186 (96%)	8 (4%)	27	43
All	All	741/770 (96%)	723 (98%)	18 (2%)	43	63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
2	B	180	VAL
2	B	191	THR
2	B	193	ILE
2	B	199	LYS
1	C	8	VAL
1	C	65	THR
1	C	124	GLU
1	C	129	ASN
1	C	157	LYS
2	D	51	ILE
2	D	54	ARG
2	D	75	LYS
2	D	103	LYS
2	D	136	LEU
2	D	139	LEU
2	D	180	VAL
2	D	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	198	HIS
1	C	67(B)	ASN
2	D	190	GLN
2	D	197	ASN

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](#)

4 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	$\# Z > 2$
4	P6G	B	301	-	18,18,18	0.37	0	17,17,17	0.34	0
5	PE7	D	301	-	21,21,21	0.39	0	19,20,20	0.23	0
3	GOL	C	301	-	5,5,5	0.20	0	5,5,5	0.20	0
3	GOL	A	301	-	5,5,5	0.26	0	5,5,5	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P6G	B	301	-	-	5/16/16/16	-
5	PE7	D	301	-	-	13/19/19/19	-
3	GOL	C	301	-	-	4/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

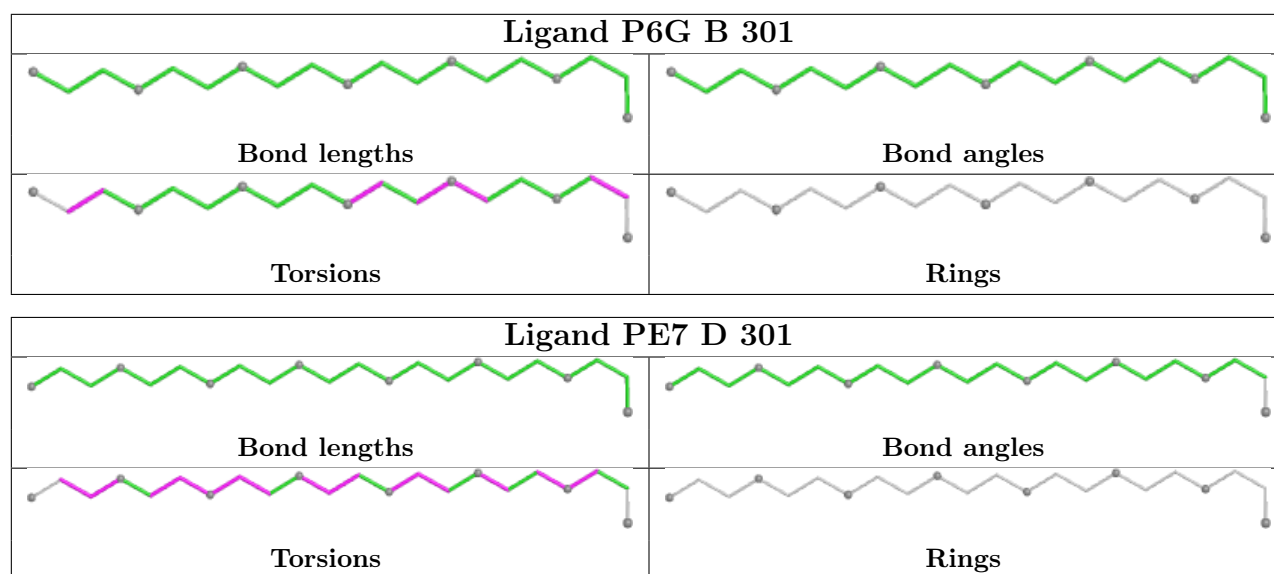
Mol	Chain	Res	Type	Atoms
5	D	301	PE7	O16-C17-C18-O19
5	D	301	PE7	O13-C14-C15-O16
3	A	301	GOL	C1-C2-C3-O3
3	C	301	GOL	O1-C1-C2-C3
3	C	301	GOL	C1-C2-C3-O3
5	D	301	PE7	O19-C20-C21-O22
3	A	301	GOL	O2-C2-C3-O3
3	C	301	GOL	O1-C1-C2-O2
4	B	301	P6G	O1-C2-C3-O4
5	D	301	PE7	C21-C20-O19-C18
4	B	301	P6G	C8-C9-O10-C11
5	D	301	PE7	C5-C6-O7-C8
4	B	301	P6G	O16-C17-C18-O19
5	D	301	PE7	C14-C15-O16-C17
3	C	301	GOL	O2-C2-C3-O3
4	B	301	P6G	C9-C8-O7-C6
5	D	301	PE7	C18-C17-O16-C15
4	B	301	P6G	C5-C6-O7-C8
5	D	301	PE7	C2-C3-O4-C5
5	D	301	PE7	C11-C12-O13-C14
5	D	301	PE7	C8-C9-O10-C11
5	D	301	PE7	C6-C5-O4-C3
5	D	301	PE7	O7-C8-C9-O10
5	D	301	PE7	O10-C11-C12-O13

There are no ring outliers.

3 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	P6G	11	0
5	D	301	PE7	18	0
3	A	301	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	211/218 (96%)	0.17	4 (1%) 66 65	25, 37, 57, 67	0
1	C	207/218 (94%)	0.57	11 (5%) 32 31	26, 42, 70, 97	0
2	B	232/236 (98%)	0.56	11 (4%) 36 36	23, 43, 74, 102	0
2	D	225/236 (95%)	0.50	15 (6%) 24 22	27, 42, 74, 110	0
All	All	875/908 (96%)	0.45	41 (4%) 36 36	23, 40, 69, 110	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	GLY	5.0
1	C	28	LEU	4.5
2	D	100(G)	PHE	4.5
1	C	70	ARG	4.1
2	B	129	THR	4.1
2	D	100(A)	ILE	4.0
1	C	67(B)	ASN	3.5
2	B	128	SER	3.5
2	D	132	GLY	3.4
2	D	100(B)	TYR	3.4
1	C	94	ARG	3.3
2	D	100(I)	GLU	3.1
2	B	132	GLY	3.1
1	C	7	TYR	3.1
2	D	78	LEU	3.1
2	D	100(H)	GLY	3.1
1	C	29	GLY	3.1
1	C	27	ALA	3.0
1	A	23	CYS	2.9
2	D	100(J)	PHE	2.8
2	D	100(E)	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	130	SER	2.7
2	D	183	PRO	2.7
2	D	125	SER	2.7
2	D	100(K)	PHE	2.7
1	C	67(A)	ILE	2.6
2	B	100(F)	SER	2.6
2	B	127	LYS	2.6
1	C	30	SER	2.6
1	A	67(A)	ILE	2.5
1	C	32	ALA	2.5
2	D	155	GLY	2.4
1	C	95(A)	GLY	2.4
2	D	100(D)	VAL	2.3
1	A	129	ASN	2.3
1	A	40	PRO	2.2
2	B	41	PRO	2.2
2	B	136	LEU	2.1
2	B	100(G)	PHE	2.1
2	D	100(C)	GLY	2.1
2	B	65	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	301	6/6	0.78	0.26	20,20,20,20	0
3	GOL	C	301	6/6	0.78	0.12	42,49,59,61	0
5	PE7	D	301	22/22	0.86	0.11	28,49,57,74	0

Continued on next page...

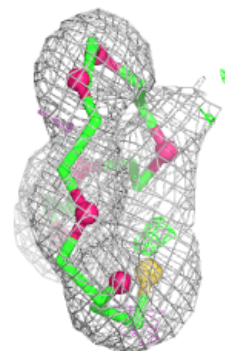
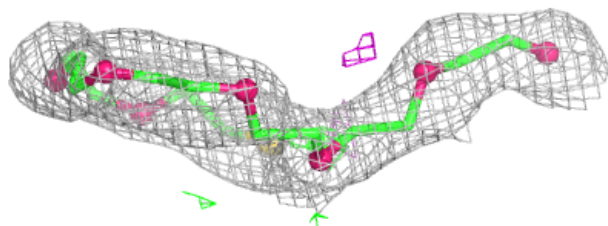
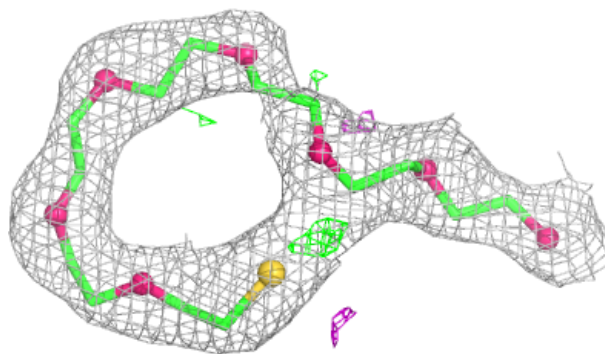
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	P6G	B	301	19/19	0.88	0.10	30,44,56,57	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

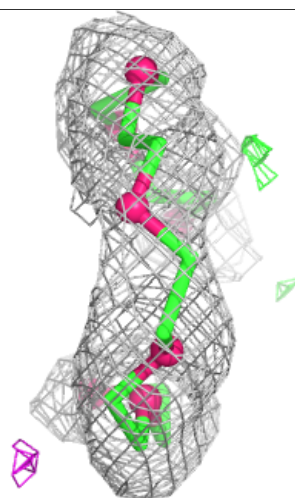
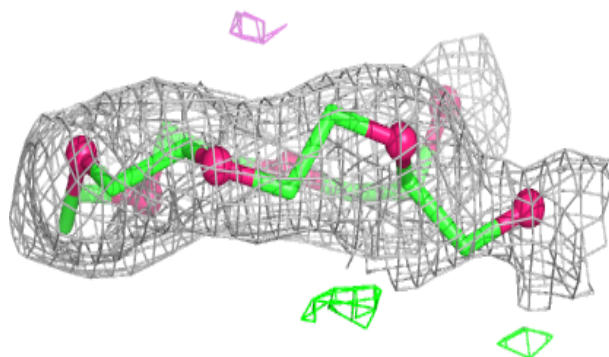
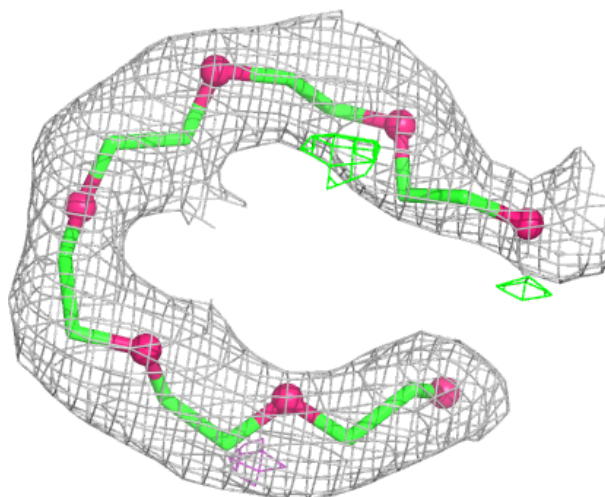
Electron density around PE7 D 301:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G B 301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.