



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:08 AM UTC

PDB ID : 4UHV / pdb_00004uhv
Title : The structure of VgrG1, the needle tip of the bacterial Type VI Secretion System
Authors : Spinola-Amilibia, M.; Davo-Siguero, I.; Ruiz, F.M.; Santillana, E.; Medrano, F.J.; Romero, A.
Deposited on : 2015-03-25
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

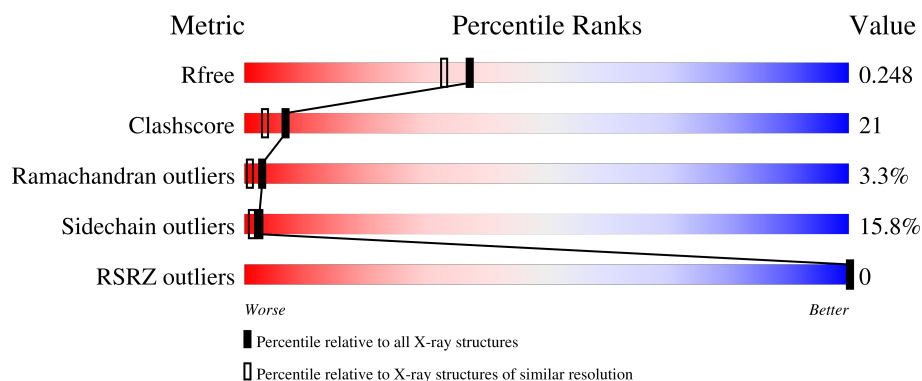
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	651	
1	B	651	

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
2	CL	B	1657	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10911 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 VGRG1, VALINE-GLYCINE REPEAT PROTEIN G1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	Se	0	3	0
			5107	3194	933	964	7	9			
1	B	645	Total	C	N	O	S	Se	0	3	0
			5109	3194	930	969	7	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	644	LEU	-	expression tag	UNP Q9I741
A	645	GLU	-	expression tag	UNP Q9I741
A	646	HIS	-	expression tag	UNP Q9I741
A	647	HIS	-	expression tag	UNP Q9I741
A	648	HIS	-	expression tag	UNP Q9I741
A	649	HIS	-	expression tag	UNP Q9I741
A	650	HIS	-	expression tag	UNP Q9I741
A	651	HIS	-	expression tag	UNP Q9I741
B	644	LEU	-	expression tag	UNP Q9I741
B	645	GLU	-	expression tag	UNP Q9I741
B	646	HIS	-	expression tag	UNP Q9I741
B	647	HIS	-	expression tag	UNP Q9I741
B	648	HIS	-	expression tag	UNP Q9I741
B	649	HIS	-	expression tag	UNP Q9I741
B	650	HIS	-	expression tag	UNP Q9I741
B	651	HIS	-	expression tag	UNP Q9I741

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	Cl	0	0
			13	13		
2	B	25	Total	Cl	0	0
			25	25		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	Na 6	0	0
3	B	7	Total 7	Na 7	0	0

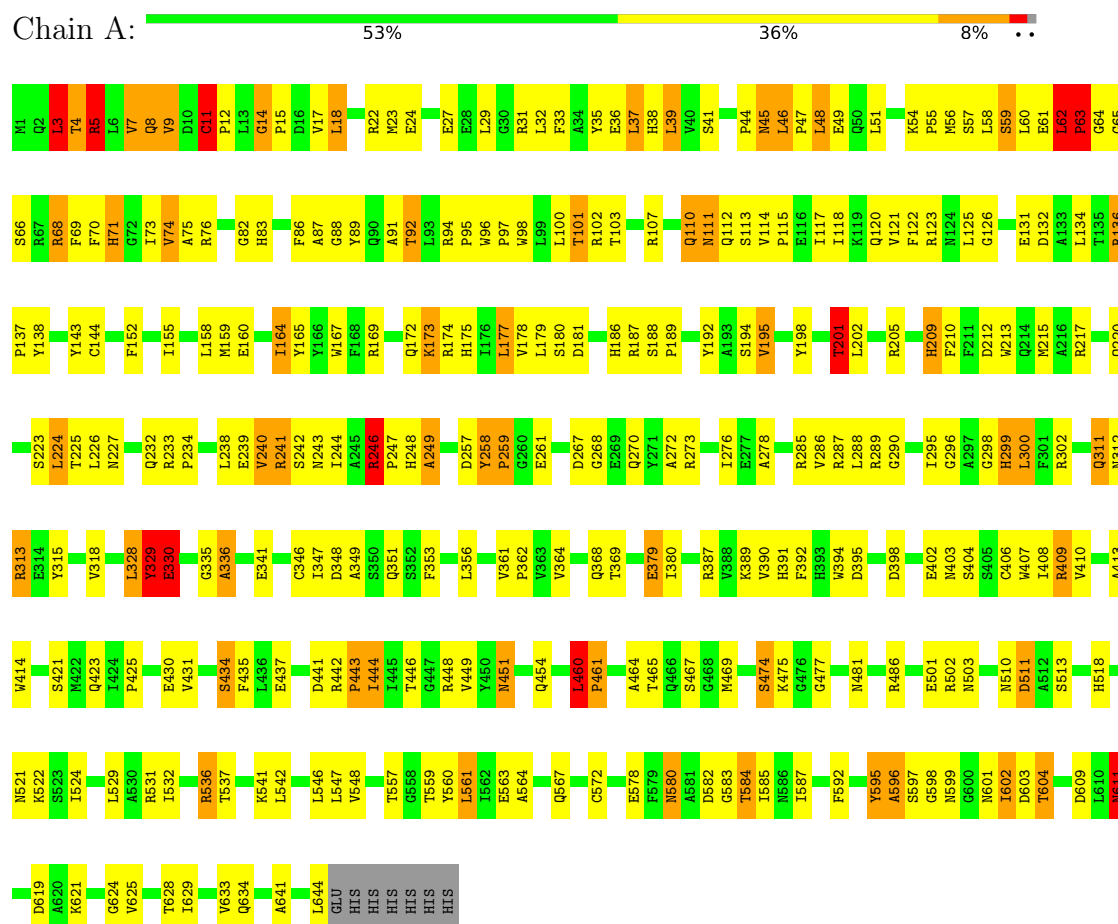
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	268	Total 268	O 268	0	0
4	B	376	Total 376	O 376	0	0

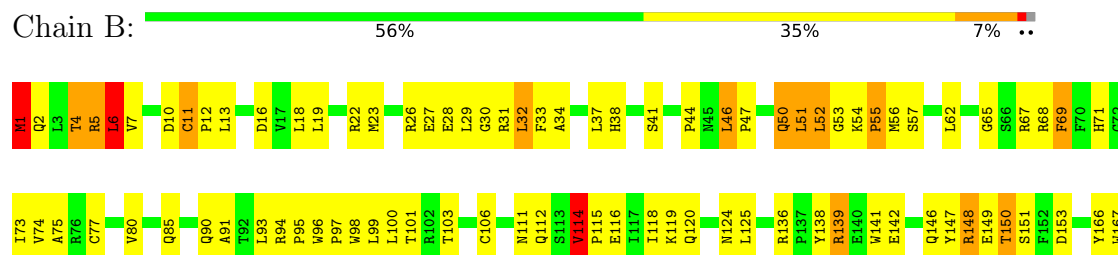
3 Residue-property plots

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: VGRG1, VALINE-GLYCINE REPEAT PROTEIN G1



• Molecule 1: VGRG1, VALINE-GLYCINE REPEAT PROTEIN G1



HIS	S553	E453	R354	F168
D594	Q454	L355	L355	R169
S555	T455	V361	E269	Q172
V556	V456	P362	R273	K173
Y560	P457	V363	I276	L176
Y560	Y458	Y363	E277	L177
E563	E459	V371	Q280	V178
E563	L460	V372	A281	L179
L570	P461	V373	Q282	S180
V571	A462	G374	H283	D181
V571	N463	P375	V286	A182
S575	A464	E378	R287	Y183
V576	T465	E379	I295	G184
V577	S474	I380	G296	A185
E578	K475	D383	A297	H186
F579	G476	G384	G298	R187
T584	G477	Y385	H299	S188
T584	T478	G386	L300	P189
I585	P479	R387	F301	G190
N586	A480	H391	G305	G191
I587	N481	F392	Y306	Y192
S588	F482	H393	P307	V195
S588	N483	W394	R308	P196
F592	M487	D395	D309	Y197
N593	E488	R396	D310	Y198
L594	D489	H397	P200	P199
L602	K490	I398	T201	P200
L608	L496	Q399	R205	P200
D609	Y497	S400	E206	T201
L610	I498	N403	D208	R209
N611	H499	W414	H209	H209
V618	A500	K417	D212	D212
D619	E501	S421	W213	W213
K623	R502	M422	Q220	Q220
G624	N510	Q423	L224	L224
V625	R520	I424	Q232	Q232
V625	S523	I427	G332	G332
I629	E528	A530	G333	G333
D630	L529	R531	G334	G334
V633	A530	I532	G335	G335
Q634	R531	N535	F340	I244
A635	I532	V540	E341	Y253
M636	F637	E540	E342	Y253
F637	P638	R541	E343	Y258
P638	P639	L542	D345	P259
P639	L644	N543	I347	V263
L644	E645	HIS	Q351	Q264
E645	HIS	L546		S265
HIS	L547	HIS		Q266
HIS	HIS			
HIS				
HIS				

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	78.62Å 78.62Å 430.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	71.73 – 2.00 71.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.0 (71.73-2.00) 94.0 (71.73-2.00)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.223 , 0.248 0.224 , 0.248	Depositor DCC
R_{free} test set	4702 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.480 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.500 for H, K, L 0.500 for K, H, -L	Depositor
Outliers	0 of 94822 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10911	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: CL, NA

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	0.72	1/5228 (0.0%)	1.07	21/7069 (0.3%)
1	B	0.77	1/5230 (0.0%)	1.12	27/7074 (0.4%)
All	All	0.75	2/10458 (0.0%)	1.09	48/14143 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	5
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	518	HIS	CA-C	7.59	1.56	1.52
1	B	510	ASN	CA-C	6.73	1.55	1.52

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	LEU	CA-C-N	18.68	143.19	119.84
1	A	460	LEU	C-N-CA	18.68	143.19	119.84
1	B	258	TYR	CA-C-N	11.43	134.13	119.84
1	B	258	TYR	C-N-CA	11.43	134.13	119.84
1	B	373	VAL	N-CA-C	9.75	123.86	108.85

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLN	Peptide
1	A	246	ARG	Peptide
1	A	258	TYR	Peptide
1	A	267	ASP	Peptide
1	A	3	LEU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5107	0	4940	228	3
1	B	5109	0	4932	202	2
2	A	13	0	0	3	0
2	B	25	0	0	8	0
3	A	6	0	0	0	0
3	B	7	0	0	0	0
4	A	268	0	0	30	1
4	B	376	0	0	29	0
All	All	10911	0	9872	431	5

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 21.

The worst 5 of 431 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:397:HIS:HD2	4:B:2179:HOH:O	1.15	1.24
1:B:258:TYR:CD2	1:B:259:PRO:HD2	1.88	1.09
1:A:11:CYS:SG	1:A:12:PRO:HD3	1.93	1.08
1:A:572:CYS:HA	4:A:2224:HOH:O	1.53	1.05
1:A:522:LYS:HE2	1:A:524:ILE:HD11	1.40	1.02

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ALA:O	4:A:2224:HOH:O[3_765]	1.76	0.44
1:A:503:ASN:ND2	1:A:511:ASP:O[3_765]	1.99	0.21
1:A:45:ASN:OD1	1:A:66:SER:OG[2_755]	2.04	0.16
1:B:465:THR:OG1	1:B:474:SER:OG[2_755]	2.12	0.08
1:B:523:SER:OG	1:B:531:ARG:NH2[2_755]	2.19	0.01

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	645/651 (99%)	519 (80%)	103 (16%)	23 (4%)	2	1
1	B	646/651 (99%)	538 (83%)	88 (14%)	20 (3%)	3	1
All	All	1291/1302 (99%)	1057 (82%)	191 (15%)	43 (3%)	3	1

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	63	PRO
1	A	64	GLY
1	A	234	PRO
1	A	249	ALA

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	539/534 (101%)	444 (82%)	95 (18%)	2	1
1	B	540/534 (101%)	465 (86%)	75 (14%)	3	2
All	All	1079/1068 (101%)	909 (84%)	170 (16%)	2	1

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	150	THR
1	B	433	VAL
1	B	205	ARG
1	B	310	ASP
1	B	490	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	83	HIS
1	B	521	ASN
1	B	243	ASN
1	B	586	ASN
1	B	429	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 51 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	635/651 (97%)	-1.10	0 100 100	10, 41, 63, 78	3 (0%)
1	B	636/651 (97%)	-1.23	0 100 100	10, 33, 54, 63	3 (0%)
All	All	1271/1302 (97%)	-1.17	0 100 100	10, 37, 59, 78	6 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	B	1707	1/1	0.97	0.06	75,75,75,75	0
2	CL	B	1655	1/1	0.98	0.06	68,68,68,68	0
2	CL	B	1656	1/1	0.98	0.05	59,59,59,59	0
2	CL	B	1648	1/1	0.98	0.07	70,70,70,70	0
3	NA	B	1663	1/1	0.98	0.06	60,60,60,60	0
3	NA	B	1711	1/1	0.98	0.07	48,48,48,48	0
3	NA	B	1712	1/1	0.98	0.04	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	1704	1/1	0.99	0.03	42,42,42,42	0
2	CL	A	1705	1/1	0.99	0.03	40,40,40,40	0
2	CL	B	1646	1/1	0.99	0.03	49,49,49,49	0
2	CL	B	1647	1/1	0.99	0.06	63,63,63,63	0
2	CL	A	1647	1/1	0.99	0.03	44,44,44,44	0
2	CL	B	1649	1/1	0.99	0.04	55,55,55,55	0
2	CL	B	1650	1/1	0.99	0.03	37,37,37,37	0
2	CL	B	1651	1/1	0.99	0.02	44,44,44,44	0
2	CL	B	1653	1/1	0.99	0.03	43,43,43,43	0
2	CL	B	1654	1/1	0.99	0.03	52,52,52,52	0
2	CL	A	1649	1/1	0.99	0.03	43,43,43,43	0
2	CL	A	1650	1/1	0.99	0.02	57,57,57,57	0
2	CL	B	1658	1/1	0.99	0.02	46,46,46,46	0
2	CL	B	1659	1/1	0.99	0.03	53,53,53,53	0
2	CL	B	1660	1/1	0.99	0.04	50,50,50,50	0
2	CL	B	1661	1/1	0.99	0.03	39,39,39,39	0
2	CL	B	1701	1/1	0.99	0.03	46,46,46,46	0
2	CL	B	1704	1/1	0.99	0.04	48,48,48,48	0
2	CL	B	1705	1/1	0.99	0.02	42,42,42,42	0
2	CL	B	1706	1/1	0.99	0.03	46,46,46,46	0
2	CL	A	1651	1/1	0.99	0.02	45,45,45,45	0
2	CL	B	1708	1/1	0.99	0.03	50,50,50,50	0
3	NA	A	1652	1/1	0.99	0.03	34,34,34,34	0
3	NA	A	1653	1/1	0.99	0.02	35,35,35,35	0
3	NA	A	1654	1/1	0.99	0.06	41,41,41,41	0
3	NA	A	1655	1/1	0.99	0.03	34,34,34,34	0
3	NA	A	1710	1/1	0.99	0.03	36,36,36,36	0
2	CL	A	1700	1/1	0.99	0.02	38,38,38,38	0
3	NA	B	1710	1/1	0.99	0.03	32,32,32,32	0
2	CL	A	1701	1/1	0.99	0.04	40,40,40,40	0
2	CL	A	1703	1/1	0.99	0.04	51,51,51,51	0
3	NA	B	1713	1/1	0.99	0.03	43,43,43,43	0
3	NA	B	1714	1/1	0.99	0.04	36,36,36,36	0
2	CL	B	1702	1/1	1.00	0.02	35,35,35,35	0
2	CL	B	1703	1/1	1.00	0.02	41,41,41,41	0
2	CL	B	1657	1/1	1.00	0.02	42,42,42,42	0
3	NA	A	1711	1/1	1.00	0.01	33,33,33,33	0
3	NA	B	1662	1/1	1.00	0.01	20,20,20,20	0
2	CL	B	1652	1/1	1.00	0.02	43,43,43,43	0
2	CL	A	1646	1/1	1.00	0.02	41,41,41,41	0
2	CL	A	1645	1/1	1.00	0.01	31,31,31,31	0
2	CL	A	1702	1/1	1.00	0.02	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	1700	1/1	1.00	0.01	26,26,26,26	0
2	CL	A	1648	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.